Access DB# 145518

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Rwong, RNC Examiner # : 69332 Date: 2/17/05
Art Unit: 1711 Phone Number 302 - 683 Serial Number: 10/723,744
Mail Box and Bldg/Room Location: 10P71 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

_____

Earliest Priority Filing Date: _____

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Product obtained by (I) + (II) + (III). Thanks.

****

STAFF USE ONLY

Searcher: _____
Searcher Phone #: _____
Searcher Location: _____
Date Searcher Picked Up: 2/25/05
Date Completed: 2/25/05
Searcher Prep & Review Time: 60
Clerical Prep Time: 40
Online Time: 325

Type of Search

NA Sequence (#) _____
AA Sequence (#) _____
Structure (#) 2
Bibliographic _____
Litigation _____
Fulltext _____
Patent Family _____
Other _____

Vendors and cost where applicable

STN ~~& 650 · 45~~
Dialog _____
Questel/Orbit _____
Dr.Link _____
Lexis/Nexis _____
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WWW/Internet _____
Other (specify) _____

PTO-1590 (8-01)

STIC Search Report
EIC 1700

STIC Database Tracking Number: 145518

TO: Duc Truong **Location: REM 10D71** **Art Unit : 1711** **February 25, 2005** **Case Serial Number: 10/723744**	**From: Usha Shrestha** **Location: EIC 1700** **REMSEN 4B28** **Phone: 571/272-3519** **usha.shrestha@uspto.gov**

Search Notes

STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact ***the EIC searcher or contact:***

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1713*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art **not found:***
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28

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Bib Data Sheet

SERIAL NUMBER	FILING DATE	CLASS	GROUP ART UNIT	ATTORNEY DOCKET NO.
10/723,744	11/26/2003 RULE	528	1711	LA/1-22803/A

APPLICANTS

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Paul Dubs, Cham, SWITZERLAND;
Roger Martin, Rheinfelden, SWITZERLAND;David Eliezer Chasan, Teaneck, NJ;
Gunnar Demme, Mahopac, NJ;
James Robbins, Satsuma, AL;

** CONTINUING DATA **********
This appln claims benefit of 60/430,228 12/02/2002

** FOREIGN APPLICATIONS **********

IF REQUIRED, FOREIGN FILING LICENSE GRANTED
** 02/26/2004

Foreign Priority claimed	STATE OR	SHEETS	TOTAL	INDEPENDENT
☐ yes ☐ no	COUNTRY	DRAWING	CLAIMS	CLAIMS
35 USC 119 (a-d) conditions met ☐ yes ☐ no ☐ Met after Allowance	SWITZERLAND	0	8	4
Verified and Acknowledged Examiner's Signature Initials				

ADDRESS
000324
CIBA SPECIALTY CHEMICALS CORPORATION
PATENT DEPARTMENT
540 WHITE PLAINS RD
P O BOX 2005
TARRYTOWN , NY
10591-9005

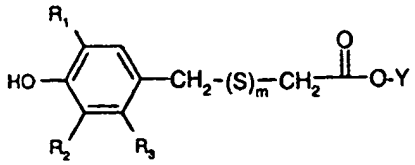
TITLE
Liquid phenolic sulphur-containing antioxidants

☐ All Fees
☐ 1.16 Fees (Filing)

Claims

1. A product obtainable by reacting

a) At least one compound



(I),

wherein

one of R_1 and R_2 independently of one another represents hydrogen or a substituent selected from the group consisting of C_1-C_{18}alkyl, phenyl, (C_1-C_4alkyl)$_{1-3}$phenyl, phenyl-C_1-C_3alkyl, (C_1-C_4alkyl)$_{1-3}$phenyl-C_1-C_3alkyl, C_5-C_{12}cycloalkyl and (C_1-C_4alkyl)$_{1-3}$$C_5$-$C_{12}$cycloalkyl;

and the other one represents a substituent selected from the group consisting of C_1-C_{18}alkyl, phenyl, (C_1-C_4alkyl)$_{1-3}$phenyl, phenyl-C_1-C_3alkyl, (C_1-C_4alkyl)$_{1-3}$phenyl-C_1-C_3alkyl, C_5-C_{12}cycloalkyl and (C_1-C_4alkyl)$_{1-3}$$C_5$-$C_{12}$cycloalkyl;

R_3 represents hydrogen or methyl;

Y represents hydrogen or C_1-C_6alkyl; and

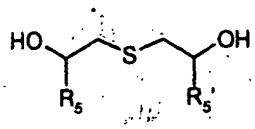
m represents zero or 1; with

b) At least one compound

$$R_4\text{-OH} \qquad \text{(II)},$$

wherein R_4 represents C_4-C_{23}alkyl; and;

c) At least one compound



(III),

wherein R_5 and R_5' independently of one another represent hydrogen or C_1-C_6alkyl.

2. A product obtainable by reacting

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 15:03:47 ON 25 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

=> d his

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                E US20040267042/PN
L1            1 S E3
                SEL  L1 RN

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L2            6 S E1-E6

     FILE 'LREGISTRY' ENTERED AT 10:22:47 ON 25 FEB 2005
L3              STR
L4              STR
L5              STR L3
L6              STR L4

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L7           34 S L5
L8              SCR 1199 OR 1312
L9              SCR 1838
L10             SCR 1332
L11          21 S L5 AND L8 AND L9 AND L10
L12             STR L5
L13          28 S L12 AND L8 AND L9 AND L10
L14           1 S L6 AND L10
L15             SCR 1774
L16           0 S L6 AND L10 AND L15
L17             SCR 1831
L18          29 S L12 AND L8 AND L9 AND L17
L19             SCR 1837 OR 1296
L20           0 S L6 AND L10 AND L19
L21           1 S L6 AND L10 AND L19 AND L15
L22             STR L6
L23             SCR 1832
L24             SCR 1312
L25          50 S L12 AND L23 AND L24
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L27             SCR 1701
L28          12 S L22 AND L15 AND L27
L29             SCR 1044
L30          50 S L12 AND L23 AND L24 AND L9 AND L29
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L33              SCR 1929
L34           50 S L12 AND L23 AND L24 AND L9 AND L29 NOT (L31 OR L33)
L35       - 49532 S L12 AND L23 AND L24 AND L9 AND L29 NOT (L31 OR L33) F
                 SAV TEMP L35 TRU723/A
L36           12 S L22 AND L15 AND L27
L37          966 S L22 AND L15 AND L27 FUL
                 SAV L37 TRU723A/A
L38            0 S L35 AND L37
                 E A/CI

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L40         2118 S L37
L41           40 S L39 AND L40
L42       794058 S ALCOHOL? OR ALC# OR ALKANOL?
L43           15 S L41 AND L42
L44           25 S L41 NOT L43
L45        13167 S L35(L)RACT/RL
L46          415 S L37(L)RACT/RL
L47           17 S L45 AND L46
L48           26 S L47 OR L43
L49           14 S L41 NOT L48
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                 SET ROLES TEXT

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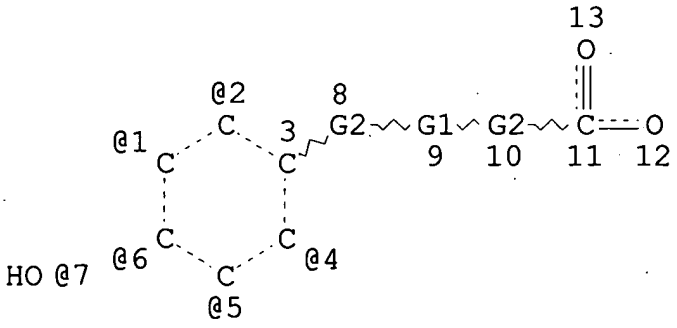


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REP G1=(0-1) S
REP G2=(1-5) C
VPA 7-4/5/6/1/2 U
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
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L24             SCR 1312
L29             SCR 1044
L31             SCR 2043
L33             SCR 1929
L35       49532 SEA FILE=REGISTRY SSS FUL L12 AND L23 AND L24 AND L9
                AND L29 NOT (L31 OR L33)

100.0% PROCESSED 378993 ITERATIONS                      49532 ANSWERS
SEARCH TIME: 00.00.10


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L22             STR

HO—G1~~~~~S~~~~~G1—OH
 1   2       4       6   7

REP G1=(1-5) C
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CONNECT IS E2  RC AT   4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   5

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 131468 ITERATIONS                       966 ANSWERS
SEARCH TIME: 00.00.02


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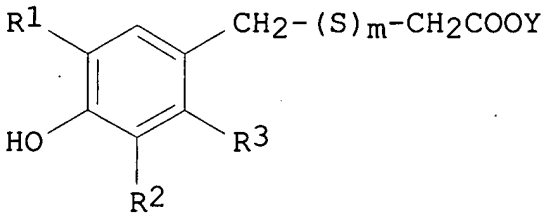
L48 ANSWER 1 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:493715 Document No. 141:56850 Thiodiethylene reaction products with **alcohols** and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and stabilizers. Camenzind, Hugo; Dubs, Paul; Martin, Roger; Chasan, David Eliezer; Demme, Gunnar; Robbins, James (Ciba Specialty Chemicals Holding Inc., Switz.). PCT Int. Appl. WO 2004050671 A1 20040617, 25 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-EP50876 20031124. PRIORITY: US 2002-PV430228 20021202.

GI



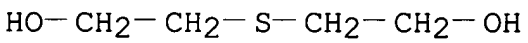
I

AB Lubricating oil antioxidants are substituted (ω-4-hydroxyphenyl)carboxylic acid derivs. synthesized by reaction of a compound of the structure R1HOR2R3C6HCH2(S)mCH2CO2Y with a C4-25-1-**alkanol** and a thiodiethylene glycol derivative of formula HO-CHR5CH2-S-CH2CHR6-OH (R5 and R6 = H and C1-6-alkyl). I is characterized by R1 and R2 = H or C1-16-alkyl, Ph, (C1-4-alkyl)1-3phenyl-, Ph-C1-3-alkyl, (C1-4-alkyl)1-3Ph-C1-3-alkyl, C5-12-cycloalkyl, and (C1-4-alkyl)1-3-C5-12- cycloalkyl; R3 = H or Me; Y = H or C1-6-alkyl; and m = 0 or 1. A preferred composition is the reaction product of thiodiethylene glycol with a

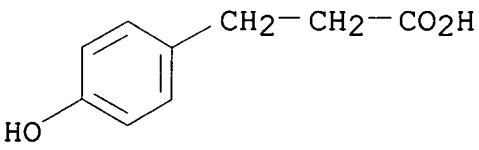
C>4-**alc**. and a substituted 5-tert-butyl-4-hydroxy-3-methyl(or tert-butyl)phenyl carboxylic acid. The compds. are not only antioxidants but also have application as thermal stabilizers and light stabilizers.

IT **111-48-8DP**, Thiodiethylene glycol, reaction products with isooctanol and Me (4-hydroxy-3,5-di-alkyl-substituted-phenyl)propanoates **501-97-3DP**, 3-(4-Hydroxyphenyl)propanoic acid, 3,5-dialkyl-substituted derivs., alkyl esters, reaction products with C4-25-**alcs**. and thiodiethylene glycol derivs. **6386-38-5DP**, reaction products with isooctanol and thiodiethylene glycol **6386-39-6DP**, reaction products with isooctanol and thiodiethylene glycol **366807-60-5DP**, 3,5-dialkyl-substituted derivs., alkyl esters, reaction products with C4-25-**alcs**. and thiodiethylene glycol derivs.
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(antioxidants; thiodiethylene reaction products with **alcs**. and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and stabilizers)

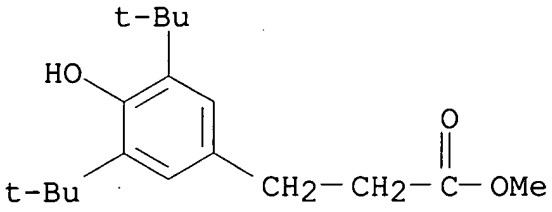
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



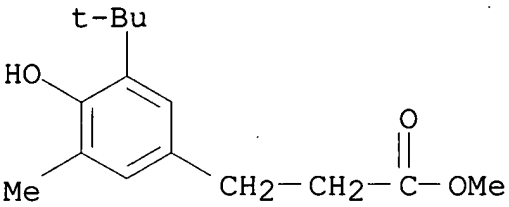
RN 501-97-3 HCAPLUS
CN Benzenepropanoic acid, 4-hydroxy- (9CI) (CA INDEX NAME)



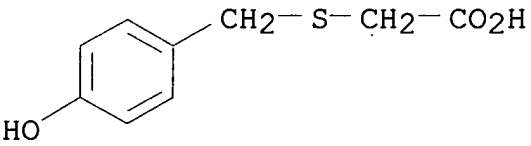
RN 6386-38-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



RN 6386-39-6 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 366807-60-5 HCAPLUS
CN Acetic acid, [[(4-hydroxyphenyl)methyl]thio]- (9CI) (CA INDEX NAME)



IC ICM C07G017-00
ICS C07C323-12; C10M135-26
CC 51-8 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 21
IT Lubricating oil additives
(antioxidants; thiodiethylene reaction products with **alcs.** and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and stabilizers)
IT Phenols, uses
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(hindered, antioxidants; thiodiethylene reaction products with **alcs.** and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and

stabilizers)

IT Stabilizing agents
(lubricating oil additives, thermal stabilizers and light stabilizers; thiodiethylene reaction products with **alcs** . and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and stabilizers)

IT **Alcohols**, uses
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(reaction products, C4-25, reaction products with thiodiethylene derivs. and hindered phenol carboxylates; thiodiethylene reaction products with **alcs**. and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and stabilizers)

IT Lubricating oil additives
(stabilizers, thermal stabilizers and light stabilizers; thiodiethylene reaction products with **alcs**. and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and stabilizers)

IT Antioxidants
Heat stabilizers
Light stabilizers
(thiodiethylene reaction products with **alcs**. and substituted (ω-4-hydroxyphenyl)carboxylates as antioxidants and stabilizers)

IT 26952-21-6DP, Exxal 8, reaction products with thiodiethylene glycol and 3-(3-tert-butyl-5-methyl(or tert-butyl)-4-hydroxyphenyl)propanoic acid Me ester
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(Exxal 8, antioxidants; thiodiethylene reaction products with **alcs**. and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and stabilizers)

IT **111-48-8DP**, Thiodiethylene glycol, reaction products with isooctanol and Me (4-hydroxy-3,5-di-alkyl-substituted-phenyl)propanoates **501-97-3DP**, 3-(4-Hydroxyphenyl)propanoic acid, 3,5-dialkyl-substituted derivs., alkyl esters, reaction products with C4-25-**alcs**. and thiodiethylene glycol derivs. **6386-38-5DP**, reaction products with isooctanol and thiodiethylene glycol **6386-39-6DP**, reaction products with isooctanol and thiodiethylene glycol **366807-60-5DP**, 3,5-dialkyl-substituted derivs., alkyl esters, reaction products with C4-25-**alcs**. and thiodiethylene glycol derivs.
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(antioxidants; thiodiethylene reaction products with

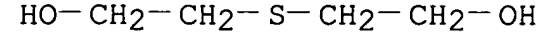
alcs. and substituted (ω-4-hydroxyphenyl)carboxylates as lubricating oil antioxidants and stabilizers)

L48 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:333874 Document No. 140:355984 Process for the preparation of phenolic carboxylic acid derivatives by enzymatic catalysis. Oehrlein, Reinhold; Baisch, Gabriele; Schoening, Kai-Uwe; Hartwig, Jemima; Mayer, Sandra Franziska (Ciba Specialty Chemicals Holding Inc., Switz.). PCT Int. Appl. WO 2004033699 A1 20040422, 36 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-EP10967 20031002. PRIORITY: EP 2002-405869 20021010.

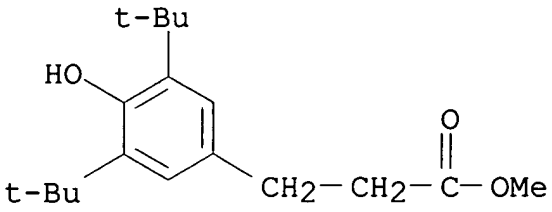
AB The present invention relates to an improved process for the preparation of phenolic carboxylic acid derivs. catalyzed by biocatalytic esterification, transesterification or amidation of a corresponding lower alkyl ester. Biocatalysis is performed in the presence of suitable enzymes, e.g. hydrolases, especially esterases, amidases, lipases and proteases.

IT **111-48-8**, Bis-(2-hydroxyethyl)sulfide **6386-38-5**, 3-(3,5-Di-tert-Butyl-4-hydroxyphenyl)propionic acid methyl ester **6386-39-6**, Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, methyl ester **38728-32-4** **84268-33-7**
RL: BCP (Biochemical process); RCT (Reactant); BIOL (Biological study); PROC (Process); **RACT (Reactant or reagent)**
(preparation of phenolic carboxylic acid derivs. by enzymic catalysis)

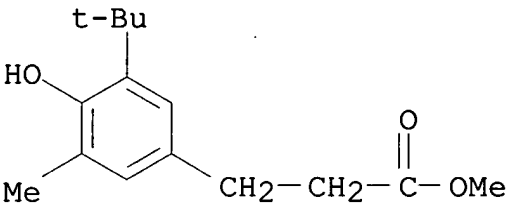
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 6386-38-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



RN 6386-39-6 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, methyl ester (9CI) (CA INDEX NAME)



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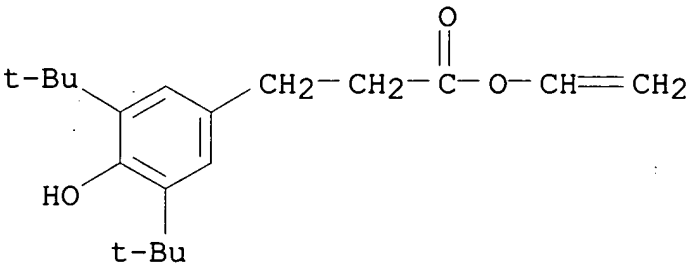
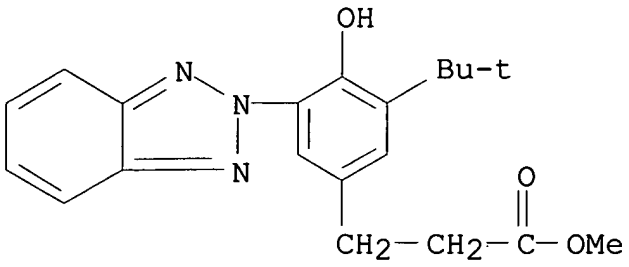
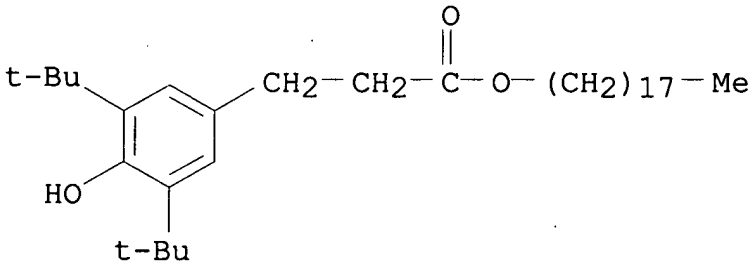


RN 84268-33-7 HCAPLUS
CN Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



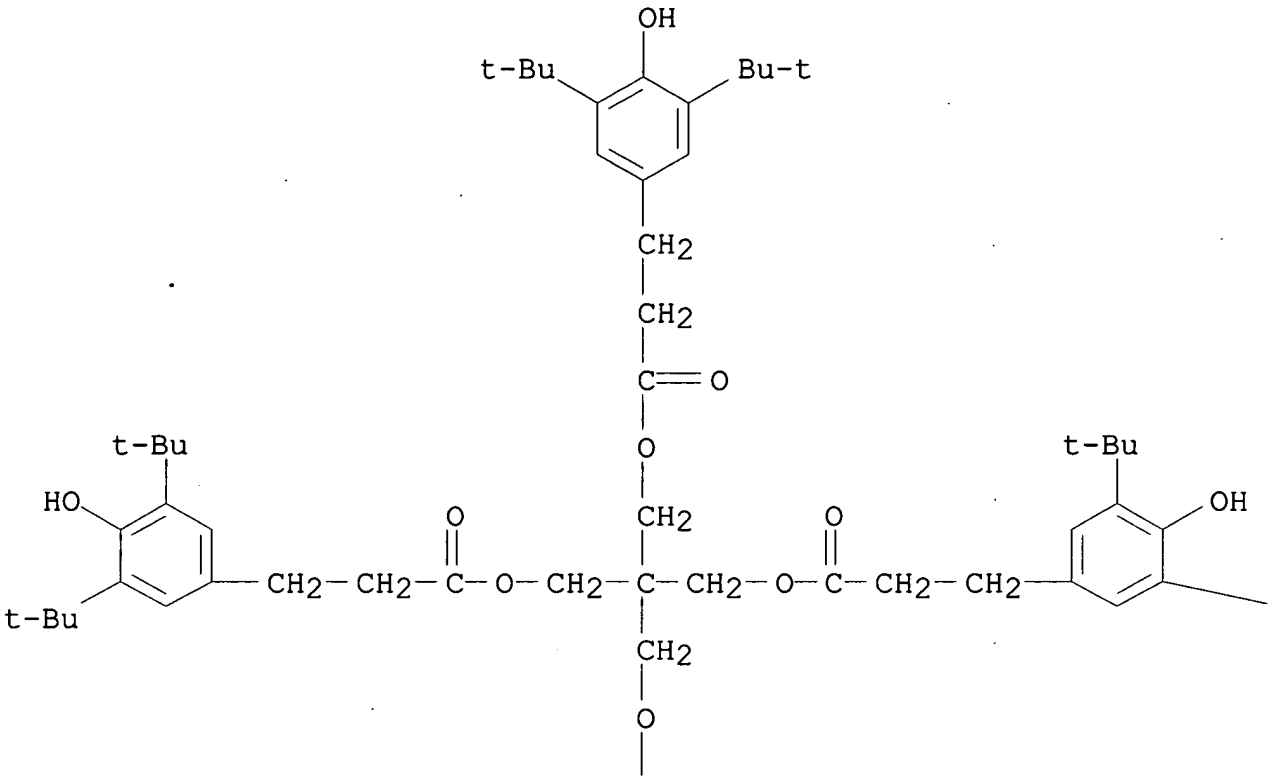
IT **2082-79-3P 6683-19-8P 34137-09-2P 34569-49-8P 35074-77-2P 36443-68-2P 36837-56-6P 41484-35-9P 84268-22-4P 84268-23-5P 144429-84-5P**
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(preparation of phenolic carboxylic acid derivs. by enzymic catalysis)

RN 2082-79-3 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (9CI) (CA INDEX NAME)



RN 6683-19-8 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2,2-bis[[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A


OH
t-Bu
Bu-t
CH2
CH2
C
O
O
t-Bu
HO
t-Bu
CH2
CH2
C
O
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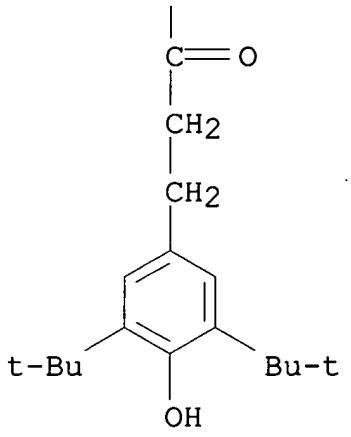
CH2
C
CH2
O
C
O
CH2
CH2
t-Bu
OH
CH2
O

PAGE 1-B

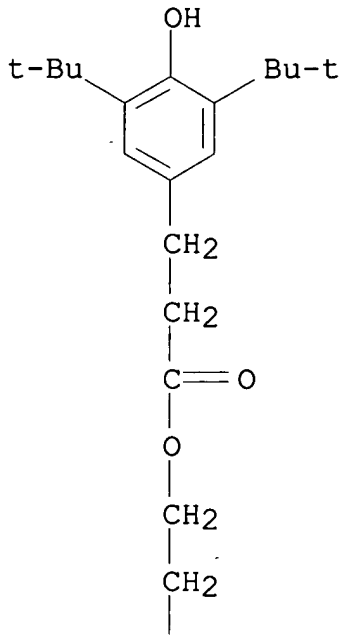
Bu-t

PAGE 2-A

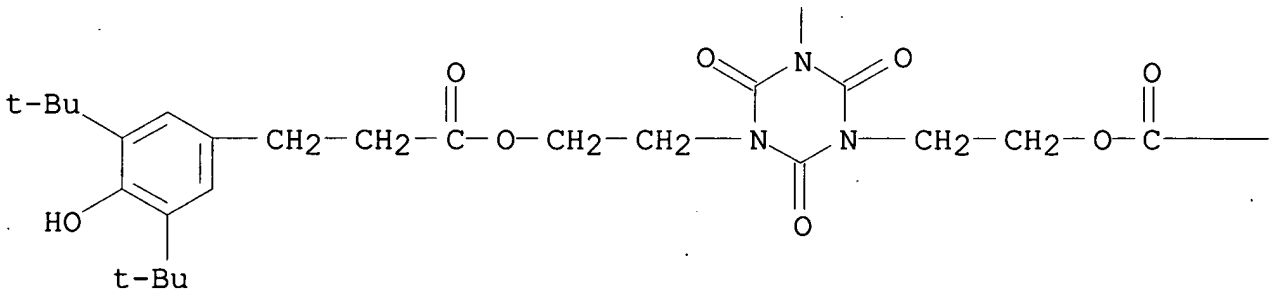


RN 34137-09-2 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, (2,4,6-trioxo-1,3,5-triazine-1,3,5(2H,4H,6H)-triyl)tri-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

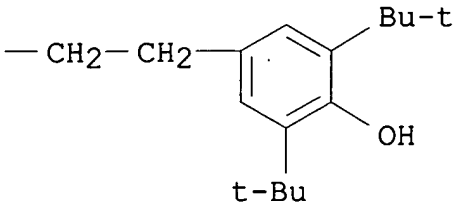
PAGE 1-A



PAGE 2-A

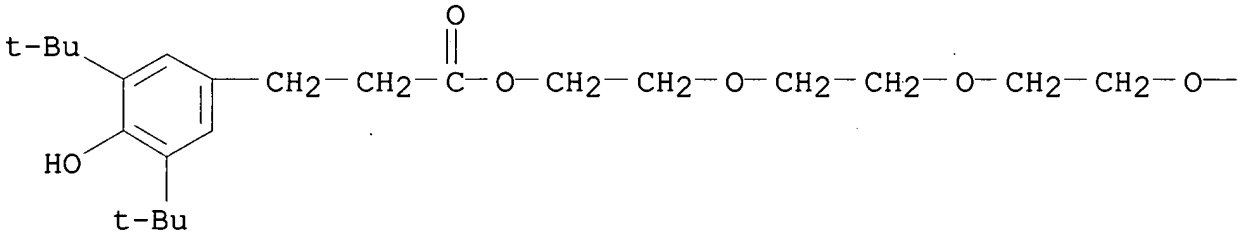


PAGE 2-B

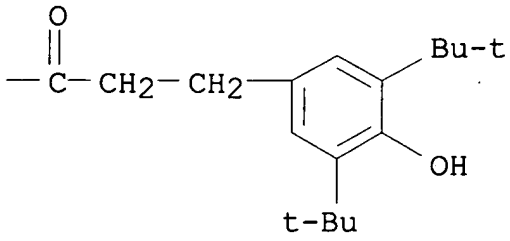


RN 34569-49-8 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester (9CI) (CA INDEX NAME)

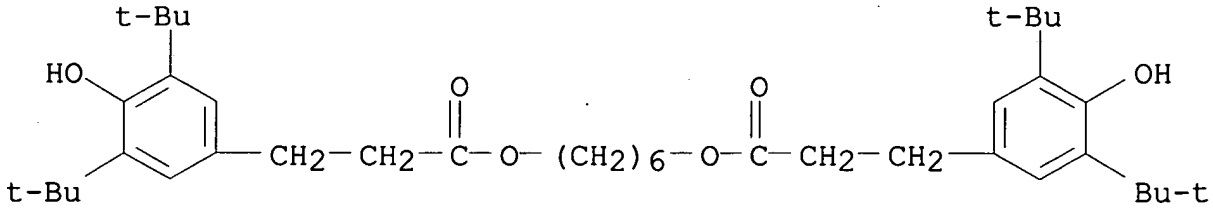
PAGE 1-A



PAGE 1-B

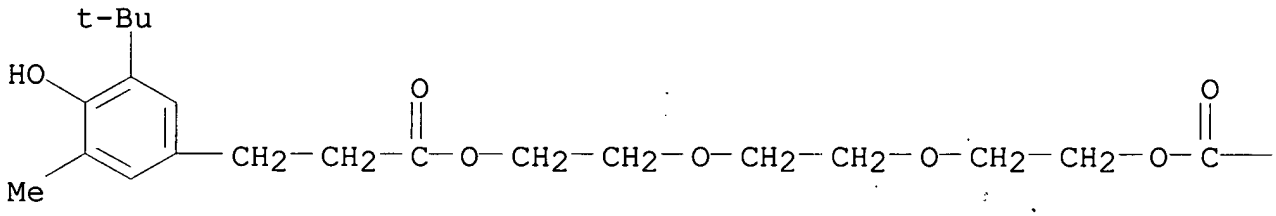


RN 35074-77-2 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)

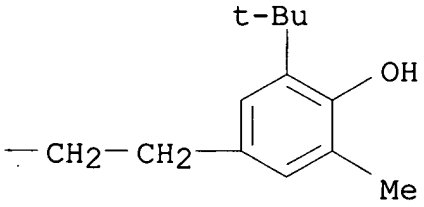


RN 36443-68-2 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester (9CI) (CA INDEX NAME)

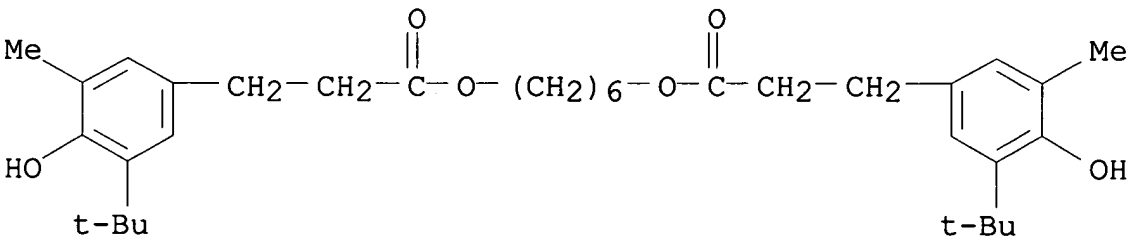
PAGE 1-A



PAGE 1-B

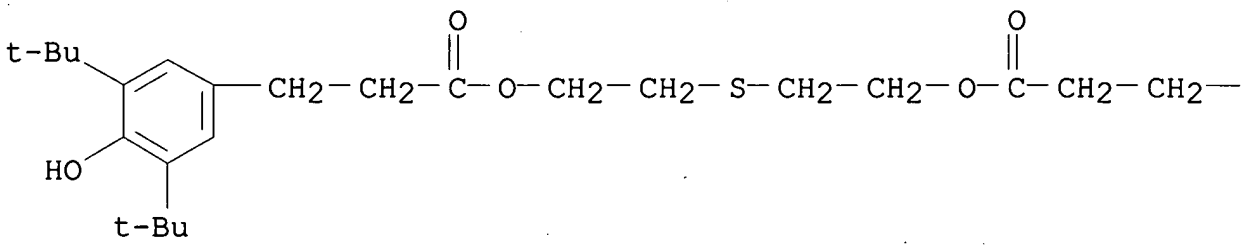


RN 36837-56-6 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)

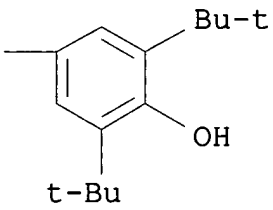


RN 41484-35-9 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

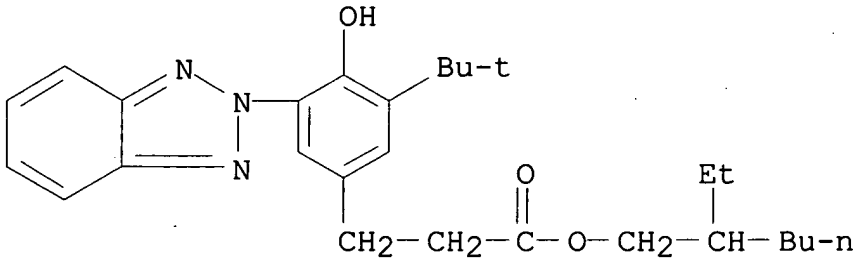
PAGE 1-A



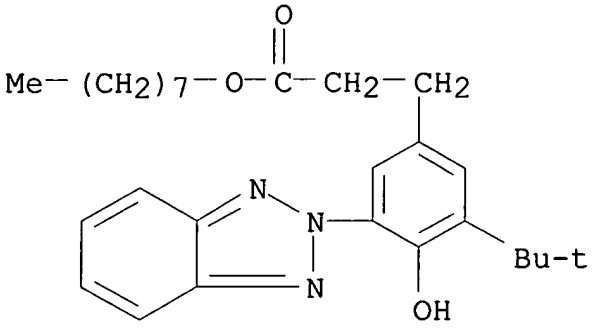
PAGE 1-B



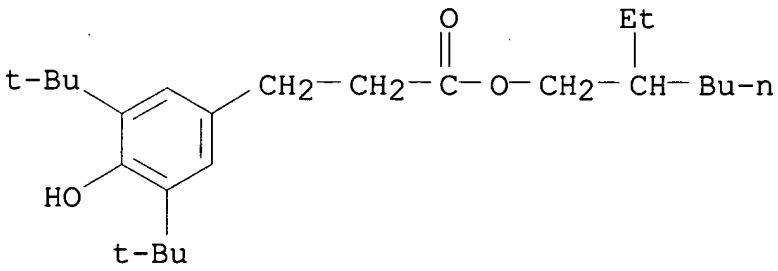
RN 84268-22-4 HCAPLUS
CN Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, 2-ethylhexyl ester (9CI) (CA INDEX NAME)



RN 84268-23-5 HCAPLUS
CN Benzenepropanoic acid, 3-(2H-benzotriazol-2-yl)-5-(1,1-dimethylethyl)-4-hydroxy-, octyl ester (9CI) (CA INDEX NAME)



RN 144429-84-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2-ethylhexyl ester (9CI) (CA INDEX NAME)

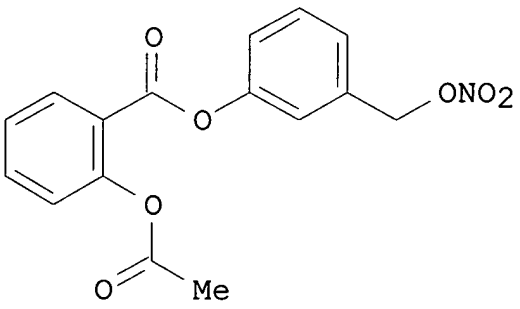


IC ICM C12P007-42
ICS C12P007-62; C12P007-22; C12P013-02
CC 16-5 (Fermentation and Bioindustrial Chemistry)
IT 104-76-7, 2-Ethyl-1-hexanol 111-42-2, Diethanolamine, reactions **111-48-8**, Bis-(2-hydroxyethyl)sulfide 111-87-5, 1-Octanol, reactions 112-27-6, Triethylene glycol 112-92-5, Stearic **alcohol** 115-77-5, Pentaerythritol, reactions 124-09-4, 1,6-Hexanediamine, reactions 629-11-8, Hexane-1,6-diol 839-90-7 **6386-38-5**, 3-(3,5-Di-tert-Butyl-4-hydroxyphenyl)propionic acid methyl ester **6386-39-6**, Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, methyl ester 7803-57-8, Hydrazine hydrate 26952-21-6, Isooctanol **38728-32-4** 83044-91-1 **84268-33-7**
RL: BCP (Biochemical process); RCT (Reactant); BIOL (Biological study); PROC (Process); **RACT (Reactant or reagent)**
(preparation of phenolic carboxylic acid derivs. by enzymic catalysis)
IT **2082-79-3P 6683-19-8P** 23128-74-7P 23328-82-7P 32687-78-8P **34137-09-2P** **34569-49-8P 35074-77-2P 36443-68-2P** **36837-56-6P** 37042-77-6P **41484-35-9P**

83044-89-7P 83044-90-0P **84268-22-4P**
84268-23-5P 144429-84-5P
RL: BMF (Bioindustrial manufacture); BPN (Biosynthetic preparation); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(preparation of phenolic carboxylic acid derivs. by enzymic catalysis)

L48 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:293592 Document No. 136:325420 Drugs for diabetes, especially type 2, comprising an antiinflammatory or analgesic drug, selected bivalent linkers, and a nitrate ester. Del Soldato, Piero (Nicox S.A., Fr.). PCT Int. Appl. WO 2002030867 A2 20020418, 66 pp. DESIGNATED STATES: W: AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CR, CU, CZ, DM, DZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-EP11665 20011009. PRIORITY: IT 2000-MI2201 20001012.

GI



II

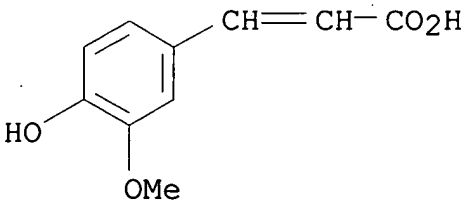
AB Useful for the treatment of diabetes, particularly type 2, are compds. or salts thereof, having the following general formula A-(B)n-(C)m-NO2 [I; wherein A = radical of a drug having an antiinflammatory or analgesic activity; B = bivalent linking group wherein the precursor must meet certain tests described in the application; C = another defined bivalent linking group; n and m = 0 or 1, provided that (n + m) = 1 or 2]. I can be used in conjunction with other antidiabetic drugs, particularly insulin. I increase the direct antidiabetic effect of insulin, and reduce complications of diabetes, particularly vascular diseases,

retinopathies, neuropathies, etc.. The values of n and m, i.e., the presence or absence of bivalent linkers B and C, alone or in combination, are based on performance of the precursors of the linkers in certain tests (no data). These tests are designated as follows: (test 4A): inhibition by > 15% of hemolysis of rat erythrocytes induced by cumene hydroperoxide; (test 5): inhibition of radical production by ≥ 50% in the oxidative degradation of . desoxyribose in aqueous Fe2+(NH4)2(SO4)2/thiobarbituric acid solution; and (test 4): inhibition by ≥ 50% of DPPH-induced radical production in MeOH solution For instance, acetylsalicylic acid chloride was esterified with 3-(hydroxymethyl)phenol (80%), followed by nitation of the resultant Ph ester with HNO3/H2SO4 (82%), to give invention compound II, which is thus the 3-(nitrooxymethyl)phenyl ester of aspirin. When tested on isolated aorta from insulin-resistant rats, compound II at a concentration of 10-4 M gave 70% vasorelaxation, relative to non-insulin-resistant controls. This effect was unchanged by the presence or absence of the irreversible NO synthetase inhibitor LNNA. In contrast, both Na nitroprussiate and the indomethacin analog of II, known NO donors, were inactive, and the antidiabetic drug metformin was inactivated by LNNA.

IT **1135-24-6**, Ferulic acid
RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(bivalent linker precursor; preparation of antidiabetic agents comprising antiinflammatory or analgesic drugs, selected bivalent linkers, and nitrate esters)

RN 1135-24-6 HCAPLUS

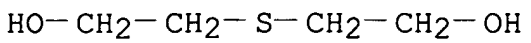
CN 2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)



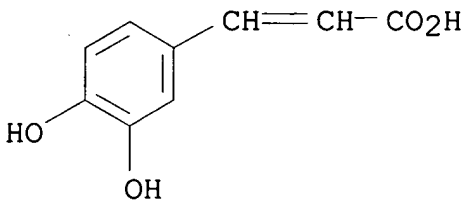
IT **111-48-8**, Thiodiethylene glycol **331-39-5**, Caffeic acid **7400-08-0**, p-Cumaric acid
RL: BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(bivalent linker precursor; preparation of antidiabetic agents

comprising antiinflammatory or analgesic drugs, selected bivalent linkers, and nitrate esters)

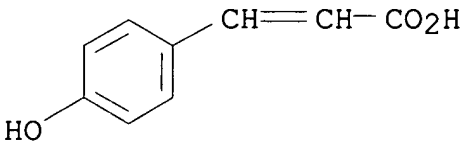
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 331-39-5 HCAPLUS
CN 2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 7400-08-0 HCAPLUS
CN 2-Propenoic acid, 3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IC ICM C07C203-04
ICS A61K031-04; A61K031-621; A61P003-10
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
IT 616-91-1, (S)-N-Acetylcysteine **1135-24-6**, Ferulic acid
RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(bivalent linker precursor; preparation of antidiabetic agents comprising antiinflammatory or analgesic drugs, selected bivalent linkers, and nitrate esters)
IT 50-81-7, Ascorbic acid, properties 52-67-5, Penicillamine 52-90-4, Cysteine, properties 56-69-9, 5-Hydroxytryptophan 56-84-8, Aspartic acid, properties 57-50-1, Saccharose, properties 60-00-4, Edetic acid, properties 60-24-2, 2-Mercaptoethanol 70-18-8, Glutathione, properties 71-00-1, Histidine, properties 77-92-9, Citric acid, properties

80-72-8, Reductic acid 89-65-6, Isoascorbic acid 105-59-9, N-Methyldiethanolamine 110-15-6, Succinic acid, properties 110-17-8, Fumaric acid, properties 110-63-4, 1,4-Butanediol, properties 111-17-1, 3,3'-Thiodipropionic acid 111-46-6, Diethylene glycol, properties **111-48-8**, Thiodiethylene glycol 117-39-5, Quercetin 120-05-8, Sulfuretin 121-34-6, Vanillic acid 121-79-9, Propyl gallate 123-31-9, Hydroquinone, properties 141-90-2, 2-Thiouracil 149-91-7, Gallic acid, properties 154-23-4, Catechin 303-45-7, Gossypol 305-84-0, L-Carnosine **331-39-5**, Caffeic acid 444-27-9, 4-Thiazolidinecarboxylic acid 458-35-5, Coniferyl **alcohol** 490-79-9, Gentisic acid 500-38-9, Nordihydroguaiaretic acid 501-94-0 520-18-3, Kaempferol 520-26-3, Hesperidin 526-84-1, Dihydroxymaleic acid 533-73-3, Hydroxyhydroquinone 584-85-0, Anserine 591-81-1, 4-Hydroxybutyric acid 635-65-4, Bilirubin, properties 824-46-4, Methoxyhydroquinone 1005-72-7, Tetrahydropyran-2,6-dimethanol 1077-28-7, Thioctic acid 1191-25-9, 6-Hydroxyhexanoic acid 1406-18-4, Vitamin E 1464-42-2, Selenomethionine 3614-08-2, Selenocysteine 3690-05-9, p-Cumaric **alcohol** 6007-86-9, Thiophene-2,5-dimethanol **7400-08-0**, p-Cumaric acid 15537-71-0, N-Acetylpenicillamine 19750-45-9, 2-Oxo-4-thiazolidinecarboxylic acid 54120-69-3, 1,4-Dioxan-2,6-dimethanol 54573-75-0, 1α-OH-Vitamin D2 55721-11-4, Secalciferol 63147-28-4, 3,5-Di-tert-butyl-4-hydroxybenzyl thioglycolate 83805-11-2, Flocalcitriol 92614-59-0, Glutathione ethyl ester 97451-46-2, Glutathione isopropyl ester 103909-75-7, 22-Oxacalcitriol 148258-92-8 326850-58-2, Tetrahydrothiopyran-2,6-dimethanol 326850-59-3, 1,4-Dithiane-2,6-dimethanol 326850-60-6, Cyclohexene-1,5-dimethanol 326850-61-7, Thiazole-2,5-dimethanol 326850-62-8, Oxazole-2,5-dimethanol 414355-30-9, 4H-Pyran-2,6-dimethanol
RL: BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(bivalent linker precursor; preparation of antidiabetic agents comprising antiinflammatory or analgesic drugs, selected bivalent linkers, and nitrate esters)

L48 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:151555 Document No. 136:200011 Preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors. Banville, Jacques; Gai, Yonghua; Johnson, Graham; Zusi, Fred Christopher; Burke, James R. (Bristol-Myers Squibb Company, USA). U.S. US 6350892 B1 20020226, 112 pp., Cont.-in-part of U.S. 6,255,496. (English). CODEN: USXXAM. APPLICATION: US 2000-507782 20000218. PRIORITY: US 1997-PV59597 19970923; US 1997-PV63518 19971027; US 1998-151002 19980910; US

1999-300111 19990427.

GI

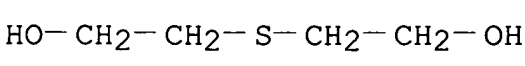
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R5 = alk(en/yn)yl, alkoxy, alkylthio, halo, hydroxy, etc.; p = 0-2; V1 = O, S0-2, NHC:O, C:ONH; R3-4 = H, Me; R1-2 = when taken together form an oxo group or R1-2 = H, OH; Y1 = O, S0-2, aza, etc.] were prepared E.g., 4-(3-hydroxypropyl)phenol was converted to Me [4-(3-methanesulfonyloxypropyl)phenoxy]acetate in 4 steps. This intermediate was reacted with N-methyl-2,2-[di(4-chlorophenyl)]ethylamine (CH3CN, NaI, 80°C, 18 h) to give the corresponding tertiary amine. The amine was treated with trifluoromethyltrimethylsilane (PhMe, -55°C) to give isolated acetal II. Hydrolysis of II (THF, HClaq) provided the example compound trifluoromethylketone isolated as the hydrochloride. Compds. I, presented in examples, showed IC50 of 1-50 μM against cPLA2.

IT **111-48-8**, 2,2'-Thiodiethanol **5597-50-2**, Methyl 3-(4-hydroxyphenyl)propionate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)

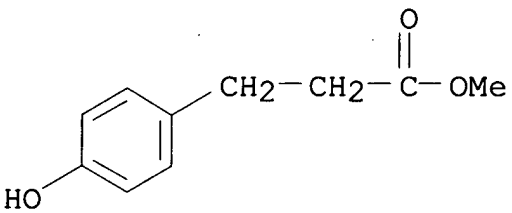
RN 111-48-8 HCAPLUS

CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

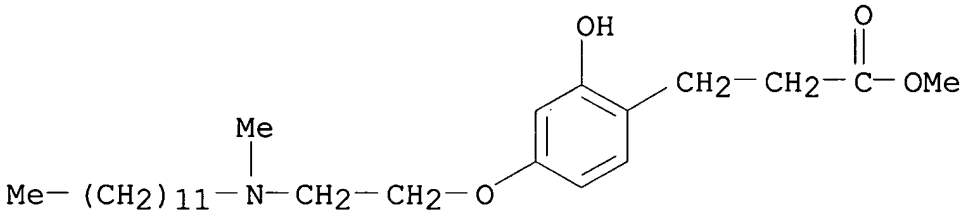


RN 5597-50-2 HCAPLUS

CN Benzenepropanoic acid, 4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



IT **221914-99-4P**, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-hydroxy-, methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)
RN 221914-99-4 HCAPLUS
CN Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



IC ICM C07F007-04
ICS C07F007-08; C07C211-00; C07C315-00; C07C317-00
NCL 556436000
CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 63
IT 51-35-4, trans-4-Hydroxy-L-proline 79-14-1, Glycolic acid, reactions 90-97-1, 4,4'-Dichlorobenzhydrol 93-35-6, 7-Hydroxycoumarin 101-76-8, 4,4'-Dichlorodiphenylmethane 105-36-2, Ethyl bromoacetate 106-41-2, 4-Bromophenol 107-08-4, 1-Iodopropane 109-83-1, 2-(Methylamino)ethanol 110-52-1, 1,4-Dibromobutane **111-48-8**, 2,2'-Thiodiethanol 112-55-0, 1-Dodecanethiol 123-08-0, 4-Hydroxybenzaldehyde 123-62-6, Propionic anhydride 124-22-1, Dodecylamine 140-88-5, 2-Propenoic acid, ethyl ester 149-73-5, Trimethyl orthoformate 383-63-1, Ethyl trifluoroacetate 421-50-1, 1,1,1-Trifluoroacetone 540-38-5, 4-Iodophenol 591-20-8, 3-Bromophenol 623-48-3, Ethyl iodoacetate 629-93-6, 1-Iodooctadecane 638-45-9, 1-Iodohexane 666-33-1, 3-Buten-2-ol, 1,1,1-trifluoro- 782-08-1, 4,4'-Dichlorobenzhydryl chloride 885-77-8, 4,4'-Dimethylbenzhydrol 1929-29-9, 3-(4-Methoxyphenyl)propionic acid 2605-67-6, Methyl (triphenylphosphoranylidene)acetate 4292-19-7, 1-Iododecane 4584-46-7, 2-(N,N-Dimethylamino)ethyl chloride hydrochloride 5292-43-3, tert-Butyl bromoacetate **5597-50-2**, Methyl 3-(4-hydroxyphenyl)propionate 6940-76-7, 1-Chloro-3-iodopropane 7311-30-0, N-Methyldodecylamine 7486-35-3, Tributylvinyltin 10138-10-0, Ethyl 4-oxobutyrate 16613-87-9, 2-

(Dodecylamino)ethanol 25666-51-7, 2-Trifluoroacetylphenol 28022-43-7, p-Chlorobenzhydrylamine 42055-15-2, 3-(Methylamino)propanol 57561-39-4, Carbamic acid, (2-hydroxyethyl)methyl-, 1,1-dimethylethyl ester 221916-21-8, 2-Butanone, 4-[3-[2-(dodecylmethylamino)ethoxy]phenyl]-1,1,1-trifluoro- 221916-22-9, 2-Butanone, 4-[2-[2-(dodecylmethylamino)ethoxy]phenyl]-1,1,1-trifluoro- 221916-23-0, 2-Butanone, 4-[4-[2-(dodecylmethylamino)ethoxy]-3-(phenylmethyl)phenyl]-1,1,1-trifluoro- 221916-24-1, Ethanone, 1-[4-[2-(dodecylmethylamino)ethoxy]-3-(phenylmethyl)phenyl]-2,2,2-trifluoro-

RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)

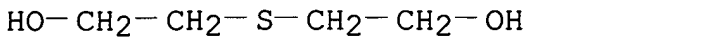
IT 1462-55-1P, Ethanol, 2-(dodecylthio)- 2474-07-9P, Ethanamine, 2-(4-bromophenoxy)-N,N-dimethyl- 2540-35-4P, Benzenepropanoic acid, 4-chloro-β-(4-chlorophenyl)- 35841-91-9P, Ethanol, 2-(dodecylmethylamino)- 35924-17-5P, Ethanol, 2-(dodecylethylamino)- 40216-83-9P, L-Proline, 4-hydroxy-, methyl ester, hydrochloride, (4R)- 54914-17-9P, Benzene, 1-(2-bromoethoxy)-4-iodo- 58859-87-3P, Benzene, 1,1'-(4-chlorobutylidene)bis[4-chloro- 87260-37-5P, 1-Propanol, 3-(dodecylmethylamino)- 95269-76-4P, Benzenepropanoic acid, 4-chloro-β-(4-chlorophenyl)-, ethyl ester 117896-99-8P, 2-Butanone, 1,1,1-trifluoro-4-(4-hydroxyphenyl)- 198990-10-2P, Carbamic acid, [2-(4-formylphenoxy)ethyl]methyl-, 1,1-dimethylethyl ester 221914-89-2P, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-, methyl ester 221914-90-5P, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-, methyl ester, hydrochloride 221914-91-6P, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-, hydrochloride 221914-92-7P, Benzenepropanoic acid, 4-[3-(dodecylmethylamino)propoxy]-, methyl ester 221914-93-8P, Benzenepropanoic acid, 4-[3-(dodecylmethylamino)propoxy]-, hydrochloride 221914-94-9P, Benzenepropanoic acid, 4-(4-bromobutoxy)-, methyl ester 221914-95-0P, Benzenepropanoic acid, 4-[4-(dodecylmethylamino)butoxy]-, methyl ester 221914-96-1P, Benzenepropanoic acid, 4-[4-(dodecylmethylamino)butoxy]-, hydrochloride 221914-97-2P, 2H-1-Benzopyran-2-one, 7-[2-(dodecylmethylamino)ethoxy]- 221914-98-3P, 2H-1-Benzopyran-2-one, 7-[2-(dodecylmethylamino)ethoxy]-3,4-dihydro- **221914-99-4P**, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-hydroxy-, methyl ester 221915-00-0P, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-methoxy-, methyl ester 221915-01-1P, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-methoxy-, hydrochloride

221915-02-2P, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-[[(trifluoromethyl)sulfonyl]oxy]-, methyl ester 221915-03-3P, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-ethenyl-, methyl ester 221915-04-4P, Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-ethenyl-, hydrochloride 221915-05-5P, Ethanol, 2-[[bis(4-chlorophenyl)methyl]methylamino]- 221915-06-6P, Benzenepropanoic acid, 4-[2-[[bis(4-chlorophenyl)methyl]methylamino]ethoxy]-, methyl ester 221915-07-7P, Benzenepropanoic acid, 4-[2-[[bis(4-chlorophenyl)methyl]methylamino]ethoxy]- 221915-08-8P, Benzenepropanamide, 4-chloro-β-(4-chlorophenyl)-N-(2-hydroxyethyl)-N-methyl- 221915-09-9P, Ethanol, 2-[[3,3-bis(4-chlorophenyl)propyl]methylamino]- 221915-10-2P, Benzenepropanoic acid, 4-[2-[[3,3-bis(4-chlorophenyl)propyl]methylamino]ethoxy]-, methyl ester 221915-11-3P, Benzenepropanoic acid, 4-[2-[[3,3-bis(4-chlorophenyl)propyl]methylamino]ethoxy]-, hydrochloride 221915-12-4P, 1-Dodecanamine, N-[2-(4-iodophenoxy)ethyl]- 221915-13-5P, Butanoic acid, 4-[dodecyl[2-(4-iodophenoxy)ethyl]amino]-, ethyl ester 221915-14-6P, Butanoic acid, 4-[dodecyl[2-[4-[(1E)-4,4,4-trifluoro-3-hydroxy-1-butenyl]phenoxy]ethyl]amino]-, ethyl ester 221915-15-7P, Butanoic acid, 4-[dodecyl[2-[4-(4,4,4-trifluoro-3-hydroxybutyl)phenoxy]ethyl]amino]-, ethyl ester 221915-16-8P, β-Alanine, N-dodecyl-N-[2-(4-iodophenoxy)ethyl]-, ethyl ester 221915-28-2P, β-Alanine, N-dodecyl-N-[2-[4-[(1E)-4,4,4-trifluoro-3-hydroxy-1-butenyl]phenoxy]ethyl]-, ethyl ester 221915-34-0P, β-Alanine, N-dodecyl-N-[2-[4-(4,4,4-trifluoro-3-hydroxybutyl)phenoxy]ethyl]-,ethylester 221915-38-4P, L-Proline, 1-dodecyl-4-hydroxy-, methyl ester, (4R)- 221915-42-0P, L-Proline, 1-dodecyl-4-(4-iodophenoxy)-, methyl ester, (4S)- 221915-48-6P, L-Proline, 1-dodecyl-4-[4-[(1E)-4,4,4-trifluoro-3-hydroxy-1-butenyl]phenoxy]-,methyl ester, (4S)- 221915-54-4P, 2-Pyrrolidinemethanol, 1-dodecyl-4-(4-iodophenoxy)-, (2S,4S)- 221915-60-2P, 2-Propenoic acid, 3-[(2S,4S)-1-dodecyl-4-(4-iodophenoxy)-2-pyrrolidinyl]-, methyl ester, (2E)- 221915-64-6P, 2-Propenoic acid, 3-[(2S,4S)-1-dodecyl-4-(4-iodophenoxy)-2-pyrrolidinyl]-, methyl ester, (2Z)- 221915-68-0P, 2-Propenoic acid, 3-[(2S,4S)-1-dodecyl-4-[4-[(1E)-4,4,4-trifluoro-3-hydroxy-1-butenyl]phenoxy]-2-pyrrolidinyl]-, methyl ester, (2E)- 221915-72-6P, 2-Pyrrolidinepropanoic acid, 1-dodecyl-4-[4-(4,4,4-trifluoro-3-hydroxybutyl)phenoxy]-, methyl ester, (2R,4S)- 221915-76-0P, Ethanone, 1-[2-[2-(dimethylamino)ethoxy]phenyl]-2,2,2-trifluoro- 221915-82-8P, Ethanone, 1-[4-[2-(dimethylamino)ethoxy]phenyl]-2,2,2-trifluoro- 221915-84-0P, Ethanamine, 2-(3-bromophenoxy)-N,N-dimethyl- 221915-86-2P, Ethanone, 1-[3-[2-(dimethylamino)ethoxy]phenyl]-2,2,2-trifluoro-

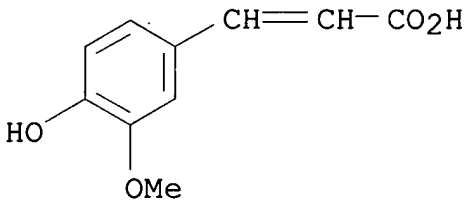
221915-87-3P, 2-Butanone, 1,1,1-trifluoro-4-(4-methoxyphenyl)-
221915-88-4P, Phenol, 4-(4,4,4-trifluoro-3,3-dimethoxybutyl)-
221915-89-5P, Benzene, 1-(2-bromoethoxy)-4-(4,4,4-trifluoro-3,3-dimethoxybutyl)- 221915-90-8P, 1-Dodecanamine, N-[2-[4-(4,4,4-trifluoro-3,3-dimethoxybutyl)phenoxy]ethyl]-
221915-91-9P, Butanoic acid, 4-[dodecyl[2-[4-(4,4,4-trifluoro-3,3-dimethoxybutyl)phenoxy]ethyl]amino]-, ethyl ester 221915-92-0P, 1-Dodecanamine, N-propyl-N-[2-[4-(4,4,4-trifluoro-3,3-dimethoxybutyl)phenoxy]ethyl]- 221915-93-1P, 1-Dodecanamine, N-hexyl-N-[2-[4-(4,4,4-trifluoro-3,3-dimethoxybutyl)phenoxy]ethyl]- 221915-94-2P, 1-Dodecanamine, N-ethyl-N-[2-[4-(4,4,4-trifluoro-3,3-dimethoxybutyl)phenoxy]ethyl]- 221915-95-3P, Carbamic acid, methyl[2-[4-[(1E)-4,4,4-trifluoro-3-oxo-1-butenyl]phenoxy]ethyl]-, 1,1-dimethylethyl ester 221915-96-4P, Carbamic acid, methyl[2-[4-(4,4,4-trifluoro-3-oxobutyl)phenoxy]ethyl]-, 1,1-dimethylethyl ester 221915-97-5P, 3-Buten-2-one, 1,1,1-trifluoro-4-(4-hydroxyphenyl)-, (3E)- 221915-98-6P, Acetic acid, [4-[(1E)-4,4,4-trifluoro-3-oxo-1-butenyl]phenoxy]-, 1,1-dimethylethyl ester 221915-99-7P, Acetic acid, [4-[(1E)-4,4,4-trifluoro-3-oxo-1-butenyl]phenoxy]- 221916-00-3P, Acetamide, N-dodecyl-2-[4-[(1E)-4,4,4-trifluoro-3-oxo-1-butenyl]phenoxy]- 221916-01-4P, Acetic acid, [4-(4,4,4-trifluoro-3-oxobutyl)phenoxy]-, 1,1-dimethylethyl ester 221916-02-5P, Acetic acid, [4-(4,4,4-trifluoro-3-oxobutyl)phenoxy]- 221916-03-6P, Benzenepropanoic acid, 4-[2-(dodecylthio)ethoxy]-, methyl ester 221916-04-7P, Benzenepropanoic acid, 4-[2-(dodecylthio)ethoxy]- 221916-05-8P, Benzene, 1,1'-[(2-bromoethoxy)methylene]bis[4-chloro- 221916-06-9P, Ethanol, 2-[[2-[bis(4-chlorophenyl)methoxy]ethyl]thio]-
221916-07-0P, Benzenepropanoic acid, 4-[2-[[2-[bis(4-chlorophenyl)methoxy]ethyl]thio]ethoxy]-, methyl ester
221916-08-1P, Benzenepropanoic acid, 4-[2-[[2-[bis(4-chlorophenyl)methoxy]ethyl]thio]ethoxy]- 221916-09-2P, 2-Butanone, 4-[4-[2-[[2-[bis(4-chlorophenyl)methoxy]ethyl]thio]ethoxy]phenyl]-1,1,1-trifluoro- 221916-10-5P, 2-Butanone, 4-[4-[2-[[2-[bis(4-chlorophenyl)methoxy]ethyl]sulfinyl]ethoxy]phenyl]-1,1,1-trifluoro- 221916-11-6P, Benzenepropanoic acid, 4-[2-[(2-hydroxyethyl)thio]ethoxy]-, methyl ester 221916-12-7P, Benzenepropanoic acid, 4-[2-[(2-hydroxyethyl)thio]ethoxy]-
221916-13-8P, Benzenepropanoic acid, 4-[2-[[2-(acetyloxy)ethyl]thio]ethoxy]- 221916-14-9P, 2-Butanone, 4-[4-[2-[[2-(acetyloxy)ethyl]thio]ethoxy]phenyl]-1,1,1-trifluoro-
221916-15-0P, Benzene, 1,1'-(4-iodobutylidene)bis[4-chloro-
221916-16-1P, Ethanol, 2-[[4,4-bis(4-chlorophenyl)butyl]thio]-
221916-17-2P, Benzenepropanoic acid, 4-[2-[[4,4-bis(4-chlorophenyl)butyl]thio]ethoxy]-, methyl ester 221916-18-3P, Benzenepropanoic acid, 4-[2-[[4,4-bis(4-chlorophenyl)butyl]thio]ethoxy]- 221916-19-4P, 2-Butanone,

4-[4-[2-[[4,4-bis(4-chlorophenyl)butyl]thio]ethoxy]phenyl]-1,1,1-trifluoro- 221916-20-7P, 2-Butanone, 4-[4-[2-[[4,4-bis(4-chlorophenyl)butyl]sulfinyl]ethoxy]phenyl]-1,1,1-trifluoro- 221916-25-2P, 2H-1-Benzopyran-2-one, 7-[2-(dodecylmethylamino)ethoxy]-3,4-dihydro-, hydrochloride 221916-26-3P, 1-Dodecanamine, N-[2-(4-iodophenoxy)ethyl]-, hydriodide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)

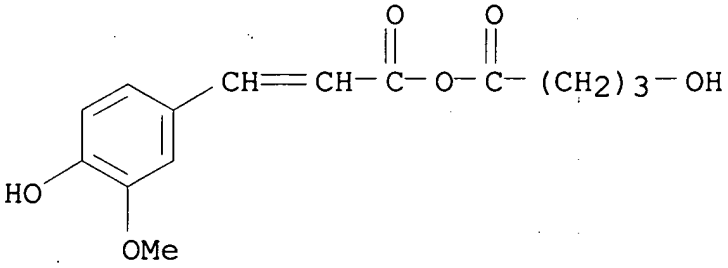
L48 ANSWER 5 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
2001:137173 Document No. 134:178396 Synthesis, activity and formulations of pharmaceutical compounds for treatment of oxidative stress and/or endothelial dysfunction. Del Soldato, Piero (Nicox S.A., Fr.). PCT Int. Appl. WO 2001012584 A2 20010222, 94 pp. DESIGNATED STATES: W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CR, CU, CZ, DM, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-EP7225 20000727. PRIORITY: IT 1999-MI1817 19990812.
AB Compds. or their salts of general formula (I): A-B-N(O)s wherein: s is an integer equal to 1 or 2; A = R-T1-, wherein R is the drug radical and T1 = (CO)t or (X)t', wherein X = O, S, NR1c, R1c is H or a linear or branched alkyl or a free valence, t and t' are integers and equal to zero or 1, with the proviso that t = 1 when t' = 0; t = 0 when t' = 1; B = -TB -X2-O- wherein TB = (CO) when t = 0, TB = X when t' = 0, X being as above defined; X2, bivalent radical, is such that the precursor drug of A and the precursor of B meet resp. the pharmacol. tests described in the description. Synthesis, activity and formulations of pharmaceutical compds. for treatment of oxidative stress and/or endothelial dysfunction are disclosed. The precursors are such as to meet the pharmacol. test reported in the description.
IT **111-48-8 1135-24-6**, Ferulic acid
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(synthesis, activity and formulations of pharmaceutical compds. for treatment of oxidative stress and/or endothelial dysfunction)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 1135-24-6 HCAPLUS
CN 2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **326850-56-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(synthesis, activity and formulations of pharmaceutical compds. for treatment of oxidative stress and/or endothelial dysfunction)
RN 326850-56-0 HCAPLUS
CN Butanoic acid, 4-hydroxy-, anhydride with 3-(4-hydroxy-3-methoxyphenyl)-2-propenoic acid (9CI) (CA INDEX NAME)



IC ICM C07C219-14
ICS C07C219-30; C07C229-42; C07C233-25; C07D219-10; C07D295-08; C07D309-30; C07D401-12; C07D471-04; C07D495-04; C07D499-68; C07H015-252; A61K031-21; C07D495-00; C07D333-00; C07D213-00
CC 26-1 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 63
IT 58-32-2, Dipyridamole 68-90-6, Benziodarone 100-55-0, Nicotinyl **alcohol** 322-79-2, Triflusal 390-64-7, Prenylamine 395-28-8, Isoxsuprine 437-74-1, Xanthinol niacinate 447-41-6, Nylidrin 456-59-7, Cyclandelate 574-77-6, Papaveroline 987-78-0, Citicoline 3611-72-1,

Clobenfurol 3703-79-5, Bamethan 5638-76-6, Betahistine 6621-47-2, Perhexiline 9005-49-6, Dalteparin, reactions 13042-18-7, Fendiline 14838-15-4, Phenylpropanolamine 22103-14-6, Bufeniode 23210-56-2, Ifenprodil 36702-83-7, Tinofedrine 37270-89-6, Nadroparin calcium 42794-76-3, Midodrine 54767-75-8, Suloctidil 57475-17-9, Brovincamine 57653-27-7, Droprenilamine 63610-08-2, Indobufen 74863-84-6, Argatroban 78919-13-8, Iloprost 81110-73-8, Acetorphan 82571-53-7, Ozagrel 89667-40-3 110140-89-1, Ridogrel 144412-49-7, Lamifiban
RL: RCT (Reactant); RACT (Reactant or reagent)
(antithrombotic; synthesis, activity and formulations of pharmaceutical compds. for treatment of oxidative stress and/or endothelial dysfunction)

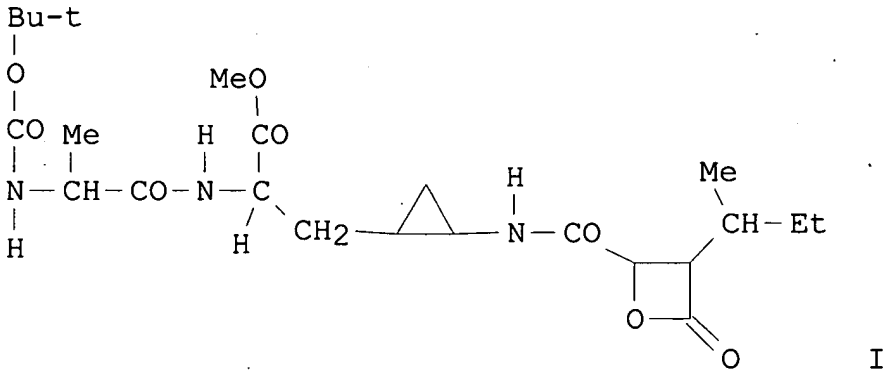
IT 69-53-4, Ampicillin 103-90-2 105-59-9, N-Methyldiethanolamine 110-63-4, 1,4-Butanediol, reactions 111-46-6, Diethylene glycol, reactions **111-48-8** 321-64-2, Tacrine 479-18-5, Diphylline 525-66-6, Propranolol 591-81-1, 4-Hydroxybutanoic acid 1005-72-7 **1135-24-6**, Ferulic acid 1191-25-9, 6-Hydroxyhexanoic acid 3447-95-8 6007-86-9, Thiophene-2,5-dimethanol 15307-86-5, Diclofenac 18559-94-9, Salbutamol 18683-91-5, Ambroxol 23214-92-8, Doxorubicin 38194-50-2, Sulindac 54120-69-3, 1,4-Dioxane-2,6-dimethanol 59277-89-3, Aciclovir 66376-36-1, Alendronic acid 75847-73-3, Enalapril 79902-63-9, Simvastatin 82964-04-3, Tolrestat 83881-51-0, Cetirizine 113665-84-2, Clopidogrel 301669-82-9 326850-58-2 326850-59-3, 1,4-Dithiane-2,6-dimethanol 326850-60-6, 3-Cyclohexene-1,3-dimethanol 326850-61-7, 2,5-Thiazoledimethanol 326850-62-8, 2,5-Oxazoledimethanol
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(synthesis, activity and formulations of pharmaceutical compds. for treatment of oxidative stress and/or endothelial dysfunction)

IT 41683-29-8P 301669-90-9P 326850-48-0P 326850-49-1P 326850-50-4P 326850-51-5P 326850-52-6P 326850-53-7P 326850-54-8P 326850-55-9P **326850-56-0P** 326850-57-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(synthesis, activity and formulations of pharmaceutical compds. for treatment of oxidative stress and/or endothelial dysfunction)

L48 ANSWER 6 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
2000:513497 Document No. 133:120677 Preparation of UCK 14A2 derivatives as proteasome inhibitors. Yamaguchi, Hiroyuki; Asai, Akira; Mizukami, Tamio; Yamashita, Yoshinori; Akinaga, Shiro; Ikeda, Shun-ichi; Kanda, Yutaka (Kyowa Hakko Kogyo Co., Ltd., Japan). PCT Int. Appl. WO 2000043000 A1 20000727, 115 pp.

DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2000-JP247 20000120. PRIORITY: JP 1999-12391 19990120; JP 1999-288539 19991008.

GI



I

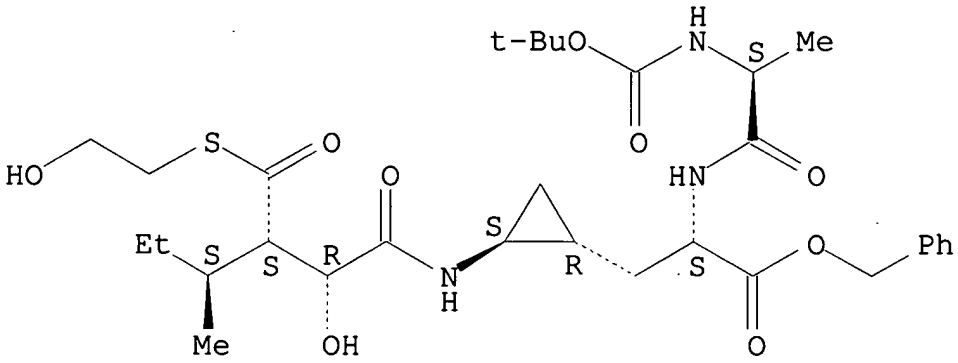
AB The title compds. R1(A)p(CH2)nX1(CH2)mX2COCH(OR3)CH(R5)COR4 [A = CHR2; m and n are each independently an integer of 0 to 10; p is 0 or 1; R1 is hydrogen, substituted or unsubstituted alkyl, substituted or unsubstituted cycloalkyl, or the like; and R2 is hydrogen, COR13, etc.; further details on R1 and R2 are given; R13 is hydroxy, substituted or unsubstituted alkoxy, etc.; X1 is a bond, substituted or unsubstituted alkylene, substituted or unsubstituted cycloalkylene, etc.; X2 is oxygen, sulfur, etc. ; R3 is hydrogen, substituted or unsubstituted alkyl, etc. ; and R4 is hydroxyl, mercapto, substituted or unsubstituted alkoxy, etc., or R3 and R4 together represent a bond; and R5 is hydrogen, substituted or unsubstituted alkyl, substituted or unsubstituted alkenyl, etc.] are prepared The title compound I in vitro showed IC50 of 0.05 μM against proteasome. Formulations are given.

IT **284483-97-2P 284483-99-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of UCK 14A2 derivs. as proteasome inhibitors)

RN 284483-97-2 HCAPLUS

CN L-Alanine, N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-3-[(1R,2S)-2-[[(2R,3S,4S)-2-hydroxy-3-[[(2-hydroxyethyl)thio]carbonyl]-4-methyl-1-oxohexyl]amino]cyclopropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

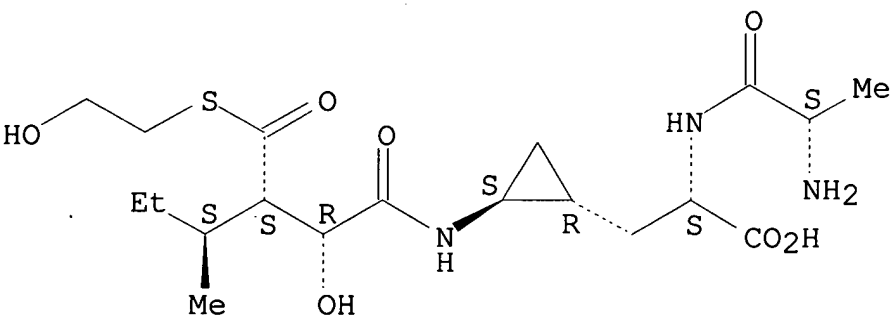


RN 284483-99-4 HCAPLUS
CN L-Alanine, L-alanyl-3-[(1R,2S)-2-[[(2R,3S,4S)-2-hydroxy-3-[[(2-hydroxyethyl)thio]carbonyl]-4-methyl-1-oxohexyl]amino]cyclopropyl]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

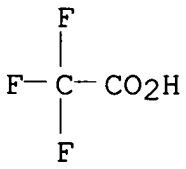
CRN 284483-98-3
CMF C19 H33 N3 O7 S

Absolute stereochemistry.



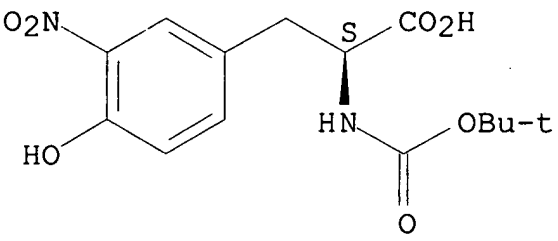
CM 2

CRN 76-05-1
CMF C2 H F3 O2



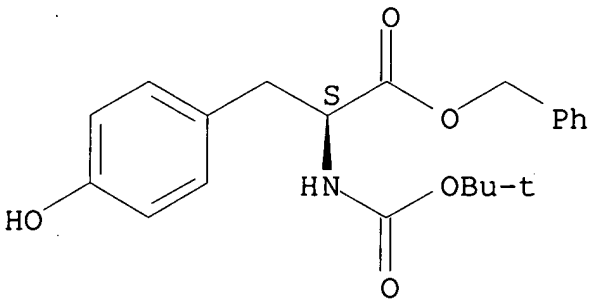
IT **5575-03-1 19391-35-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of UCK 14A2 derivs. as proteasome inhibitors)
RN 5575-03-1 HCAPLUS
CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-3-nitro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 19391-35-6 HCAPLUS
CN L-Tyrosine, N-[(1,1-dimethylethoxy)carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K031-215
ICS A61K031-27; A61K031-337; A61K031-497; A61K031-501; A61K031-506; C07C271-22; C07C237-10; C07C327-22; C07C327-28; C07D305-12; C07D405-12; A61P043-00; A61P035-00

CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 63

IT 284483-13-2P 284483-15-4P 284483-16-5P 284483-18-7P
284483-19-8P 284483-21-2P 284483-22-3P 284483-23-4P
284483-24-5P 284483-26-7P 284483-27-8P 284483-30-3P
284483-31-4P 284483-32-5P 284483-33-6P 284483-34-7P
284483-35-8P 284483-36-9P 284483-38-1P 284483-39-2P
284483-41-6P 284483-42-7P 284483-43-8P 284483-45-0P
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284483-54-1P 284483-55-2P 284483-56-3P 284483-57-4P
284483-58-5P 284483-59-6P 284483-60-9P 284483-61-0P
284483-62-1P 284483-63-2P 284483-64-3P 284483-65-4P
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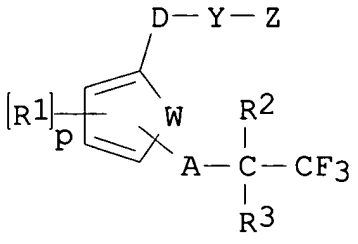
284483-72-3P 284483-73-4P 284483-75-6P 284483-76-7P
284483-77-8P 284483-78-9P 284483-79-0P 284483-80-3P
284483-81-4P 284483-82-5P 284483-84-7P 284483-85-8P
284483-87-0P 284483-88-1P 284483-90-5P 284483-91-6P
284483-93-8P 284483-94-9P 284483-96-1P **284483-97-2P**
284483-99-4P 284484-00-0P 284484-01-1P 284484-02-2P
284484-03-3P 284484-04-4P 284484-05-5P 284484-06-6P
284484-07-7P 284484-08-8P 284484-09-9P 284484-10-2P
284484-11-3P 284484-12-4P 284484-13-5P 284484-14-6P
284484-15-7P 284484-17-9P 285561-46-8P 285561-47-9P
285561-48-0P 285561-49-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of UCK 14A2 derivs. as proteasome inhibitors)

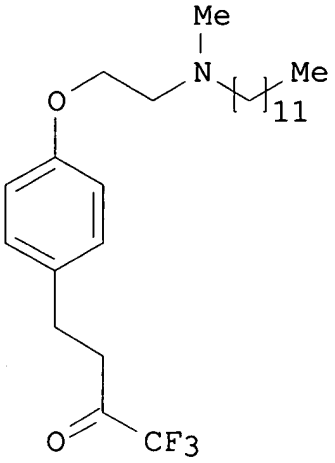
IT 60-24-2, Mercaptoethanol 64-18-6, Formic acid, reactions 70-11-1, 2-Bromoacetophenone 71-36-3, Butyl **alcohol**, reactions 74-88-4, Methyl iodide, reactions 75-08-1, Ethanethiol 77-76-9, 2,2-Dimethoxypropane 93-97-0, Benzoic anhydride 98-09-9, Benzenesulfonyl chloride 98-97-5, 2-Pyrazinecarboxylic acid 100-39-0, Benzyl bromide 100-46-9, Benzylamine, reactions 100-49-2, Cyclohexylmethanol 100-51-6, Benzenemethanol, reactions 100-63-0, Phenylhydrazine 106-95-6, Allyl bromide, reactions 108-24-7, Acetic anhydride 109-73-9, Butylamine, reactions 110-91-8, Morpholine, reactions 118-31-0, 1-Naphthalenemethylamine 124-63-0, Methanesulfonyl chloride 383-63-1, Ethyl trifluoroacetate 456-41-7, 3-Fluorobenzyl bromide 501-53-1, Benzyl chloroformate 513-38-2, 1-Iodo-2-methylpropane 622-78-6, Benzyl isothiocyanate 624-76-0, 2-Iodoethanol 691-84-9 939-26-4, 2-(Bromomethyl)naphthalene 1458-98-6, 3-Bromo-2-methylpropene 1499-21-4, Diphenylphosphinic chloride 1795-48-8, Isopropyl isocyanate 2916-68-9, 2-(Trimethylsilyl)ethanol 3173-56-6,

Benzyl isocyanate 5515-01-5, Benzyl 6-aminocaproate **5575-03-1** 5798-78-7, p-Bromobenzyl chloroformate 7554-28-1 13057-17-5, Bromomethyl methyl ether 15761-38-3, N-(tert-Butyloxycarbonyl)-L-alanine 17831-01-5, L-Alanine benzyl ester 18107-18-1, Trimethylsilyldiazomethane **19391-35-6** 21887-64-9 22509-74-6, N-Carbethoxyphthalimide 24424-99-5, Di-tert-butyl dicarbonate 24463-19-2, 9-(Chloromethyl)anthracene 51644-96-3 66617-58-1 98946-18-0, tert-Butyl 2,2,2-trichloroacetimidate 120821-20-7 142663-85-2 158896-17-4 177019-47-5 189871-55-4 189871-57-6 284484-18-0 284484-19-1 284484-20-4 284484-21-5 284484-22-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of UCK 14A2 derivs. as proteasome inhibitors)

L48 ANSWER 7 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1999:231488 Document No. 130:267208 Preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors. Banville, Jacques; Gai, Yonghua; Johnson, Graham; Zusi, Fred Christopher; Burke, James R. (Bristol-Myers Squibb Company, USA). PCT Int. Appl. WO 9915129 A2 19990401, 257 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US19426 19980917. PRIORITY: US 1997-59597 19970923; US 1997-63518 19971027.
GI



I



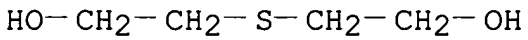
II

AB The title compds. [I; W = CH:CH, CH:N, O, S; R1 = alkyl, alkenyl, alkynyl, etc.; p =0=2; a = V(R4)n; R4 = alkyl; n = 0-6; R2 and R3 when taken together form an oxo group; R2, R3 = H, OH; V = O, S, SO, etc.; D = (CH2)m, a bond; m = 1-6; Y = O, S, SO, etc.; Z = (CH2)qC(R5)(R6)BNR7R8; B = C(:X), OC(:X), SO2, etc.; X = S, O; q = 1-6; R5, R6 = H, C1-18 alkyl; R7, R8 = H, (un)substituted C1-18 alkyl, etc.], selective inhibitors of the cPLA2 enzymes which are of use in controlling a wide variety of inflammatory diseases, were prepared Thus, a 4-step synthesis of the title compound II, starting with iodododecane and 2-(methylamino)ethanol, was given. Compds. I, presented in examples, showed IC50 of 1-50 μM against cPLA2.

IT **111-48-8**, 2,2'-Thiodiethanol **5597-50-2**, Methyl 3-(4-hydroxyphenyl)propionate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)

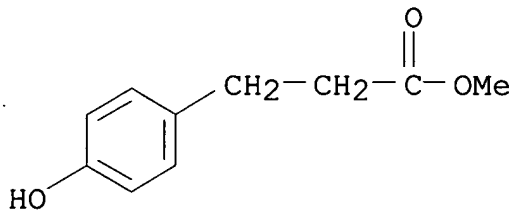
RN 111-48-8 HCAPLUS

CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

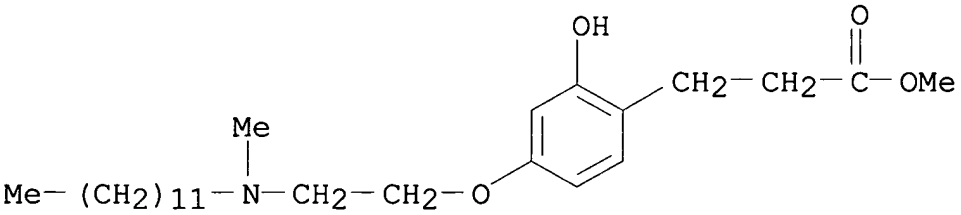


RN 5597-50-2 HCAPLUS

CN Benzenepropanoic acid, 4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



IT **221914-99-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)
RN 221914-99-4 HCAPLUS
CN Benzenepropanoic acid, 4-[2-(dodecylmethylamino)ethoxy]-2-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



IC ICM A61K
CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1
IT 51-35-4, trans-4-Hydroxy-L-proline 79-14-1, Glycolic acid, reactions 90-97-1, 4,4'-Dichlorobenzhydrol 93-35-6, 7-Hydroxycoumarin 101-76-8, 4,4'-Dichlorodiphenylmethane 105-36-2, Ethyl bromoacetate 106-41-2, 4-Bromophenol 107-08-4, 1-Iodopropane 109-83-1, 2-(Methylamino)ethanol 110-52-1, 1,4-Dibromobutane **111-48-8**, 2,2'-Thiodiethanol 112-55-0, 1-Dodecanethiol 123-08-0, 4-Hydroxybenzaldehyde 123-62-6, Propionic anhydride 124-22-1, Dodecylamine 140-88-5 149-73-5, Trimethyl orthoformate 383-63-1, Ethyl trifluoroacetate 421-50-1, 1,1,1-Trifluoroacetone 540-38-5, 4-Iodophenol 591-20-8, 3-Bromophenol 623-48-3, Ethyl iodoacetate 629-93-6, 1-Iodooctadecane 638-45-9, 1-Iodohexane 666-33-1 782-08-1, 4,4'-Dichlorobenzhydryl chloride 885-77-8, 4,4'-Dimethylbenzhydrol 1929-29-9, 3-(4-Methoxyphenyl)propionic acid 2605-67-6, Methyl (triphenylphosphoranylidene)acetate 4292-19-7, 1-Iodododecane 4584-46-7, 2-(N,N-Dimethylamino)ethyl chloride hydrochloride 5292-43-3, tert-Butyl bromoacetate

5597-50-2, Methyl 3-(4-hydroxyphenyl)propionate 6940-76-7, 1-Chloro-3-iodopropane 7311-30-0, N-Methyldodecylamine 7486-35-3, Tributylvinyltin 10138-10-0, Ethyl 4-oxobutyrate 16613-87-9, 2-(Dodecylamino)ethanol 25666-51-7, 2-Trifluoroacetylphenol 28022-43-7, p-Chlorobenzhydrylamine 42055-15-2, 3-(Methylamino)propanol 57561-39-4 221916-21-8 221916-22-9 221916-23-0 221916-24-1
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)

IT 1462-55-1P 2474-07-9P 2540-35-4P 35841-91-9P 35924-17-5P 40216-83-9P 54914-17-9P 58859-87-3P 87260-37-5P 95269-76-4P 117896-99-8P 198990-10-2P 221914-89-2P 221914-90-5P 221914-91-6P 221914-92-7P 221914-93-8P 221914-94-9P 221914-95-0P 221914-96-1P 221914-97-2P 221914-98-3P **221914-99-4P** 221915-00-0P 221915-01-1P 221915-02-2P 221915-03-3P 221915-04-4P 221915-05-5P 221915-06-6P 221915-07-7P 221915-08-8P 221915-09-9P 221915-10-2P 221915-11-3P 221915-12-4P 221915-13-5P 221915-14-6P 221915-15-7P 221915-16-8P 221915-28-2P 221915-34-0P 221915-38-4P 221915-42-0P 221915-48-6P 221915-54-4P 221915-60-2P 221915-64-6P 221915-68-0P 221915-72-6P 221915-76-0P 221915-82-8P 221915-84-0P 221915-86-2P 221915-87-3P 221915-88-4P 221915-89-5P 221915-90-8P 221915-91-9P 221915-92-0P 221915-93-1P 221915-94-2P 221915-95-3P 221915-96-4P 221915-97-5P 221915-98-6P 221915-99-7P 221916-00-3P 221916-01-4P 221916-02-5P 221916-03-6P 221916-04-7P 221916-05-8P 221916-06-9P 221916-07-0P 221916-08-1P 221916-09-2P 221916-10-5P 221916-11-6P 221916-12-7P 221916-13-8P 221916-14-9P 221916-15-0P 221916-16-1P 221916-17-2P 221916-18-3P 221916-19-4P 221916-20-7P 221916-25-2P 221916-26-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of O-substituted 4-(4-hydroxyphenyl)-1,1,1-trifluoro-2-butanones as selective cPLA2 inhibitors)

L48 ANSWER 8 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1999:227967 Document No. 130:283677 Process for the preparation of substituted hydroxyhydrocinnamate esters. Ross, John R.; Schultz, Michael E.; Dubuis, Benoit; Kung, Peter (Ciba Specialty Chemicals Corporation, USA). U.S. US 5892097 A 19990406, 5 pp. (English). CODEN: USXXAM. APPLICATION: US 1997-862034 19970522.

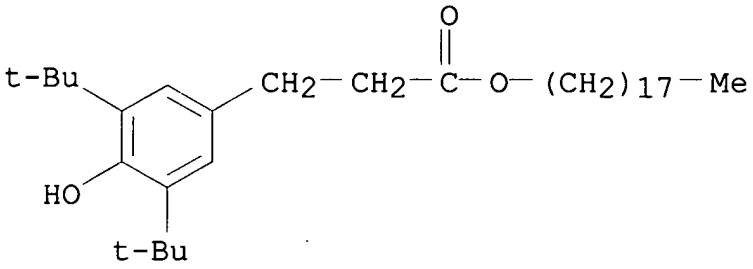
AB The transesterification of substituted lower alkyl hydroxyhydrocinnamates with a higher **alc**. or a polyol is

greatly facilitated by the use of a trace amount of a tin catalyst. In many cases, the amount of the catalyst is so small that it is unnecessary to remove it from the final product by distillation of said product.

IT **2082-79-3P**, n-Octadecyl 3,5-di-tert-butyl-4-hydroxyhydrocinnamate **6386-68-1P 6683-19-8P 6997-02-0P 13417-12-4P 15229-61-5P 34569-49-8P 35074-77-2P 41484-35-9P 53926-93-5P 85278-90-6P 146598-26-7P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(process for the preparation of substituted hydroxyhydrocinnamate esters)

RN 2082-79-3 HCAPLUS

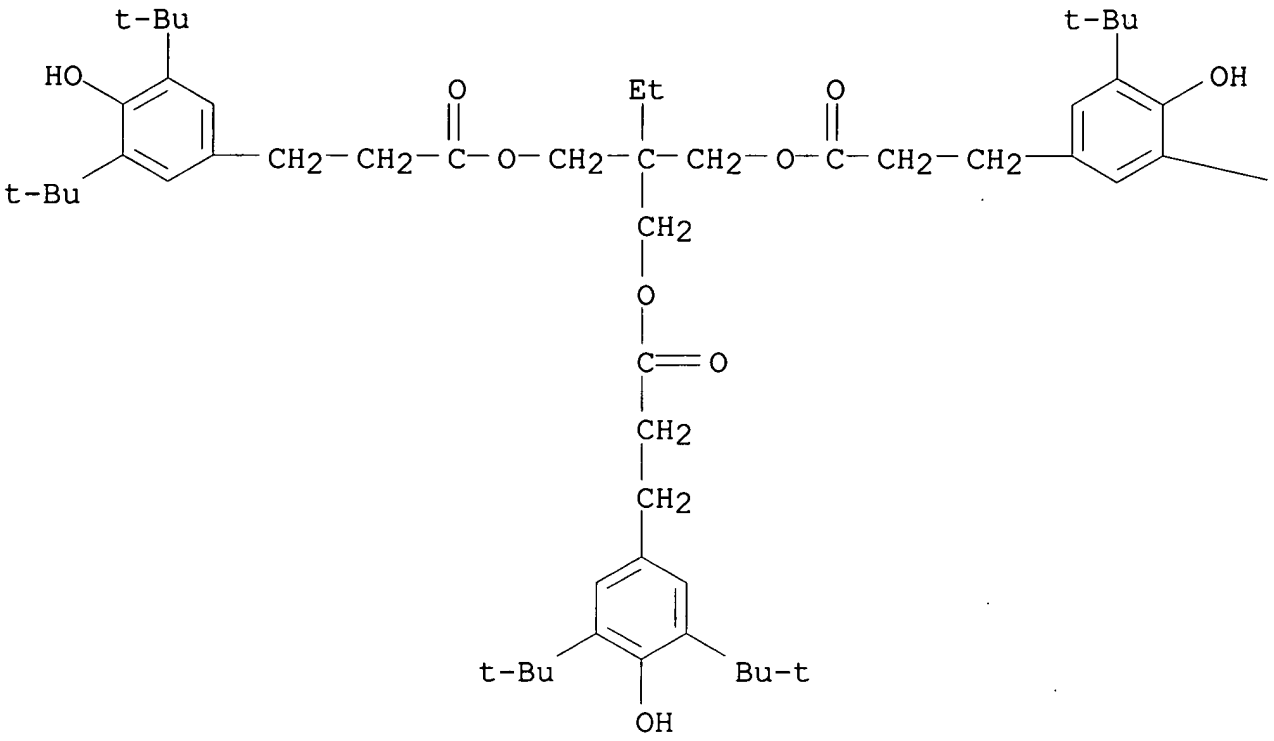
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (9CI) (CA INDEX NAME)



RN 6386-68-1 HCAPLUS

CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2-[[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]methyl]-2-ethyl-1,3-propanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

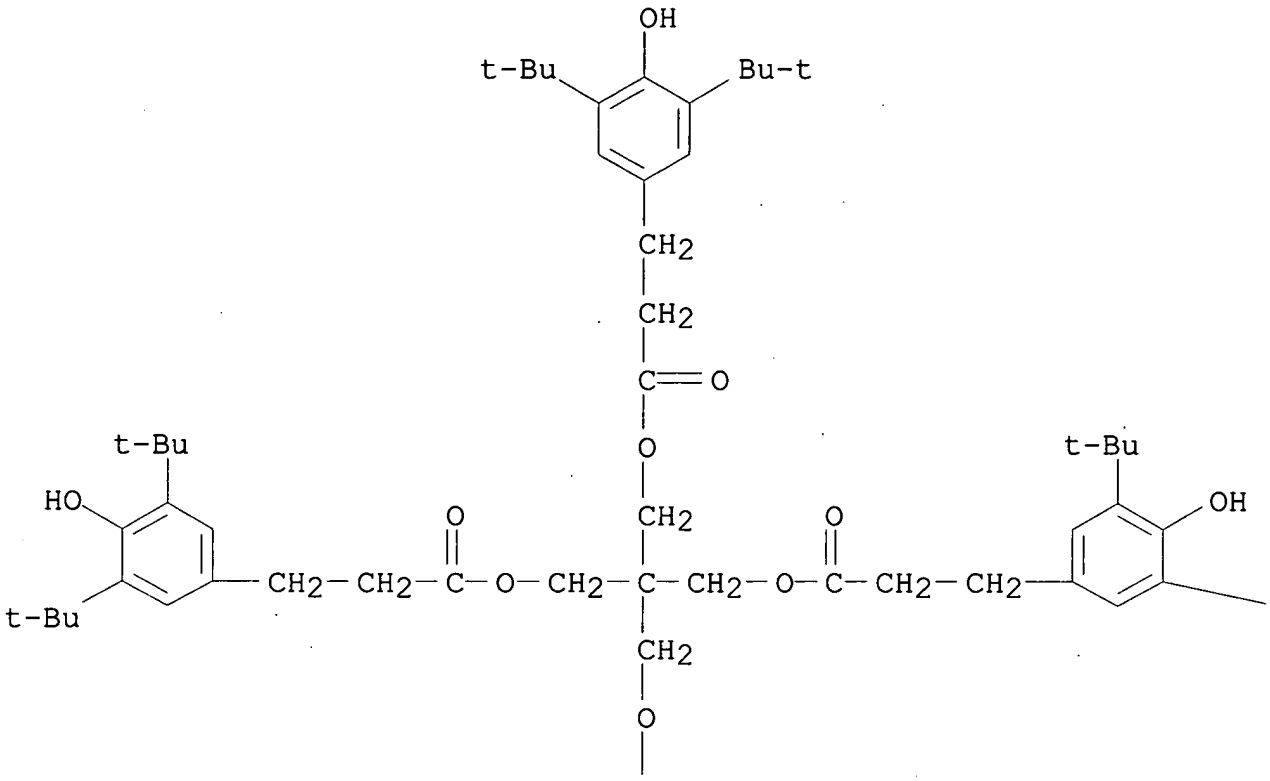


PAGE 1-B

Bu-t

RN 6683-19-8 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2,2-bis[[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A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CH2
C
O
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CH2
CH2
C
O
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CH2
C
CH2
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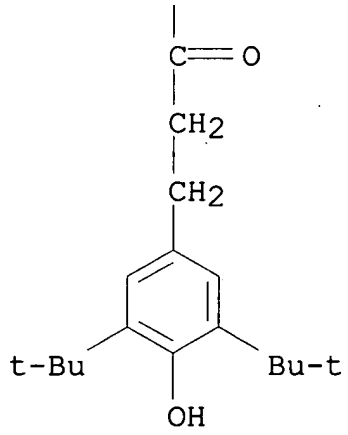
C
O
CH2
CH2
t-Bu
OH
CH2
O

PAGE 1-B

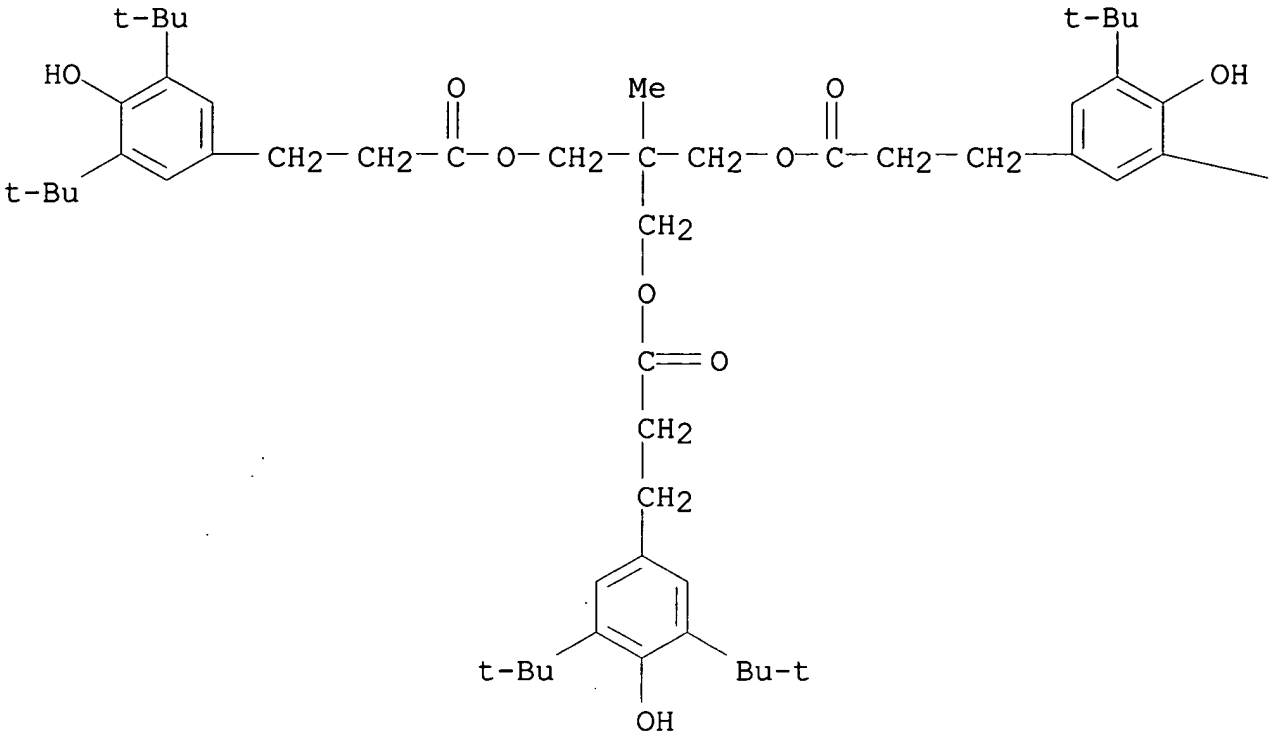
Bu-t

PAGE 2-A



RN 6997-02-0 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2-[[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]methyl]-2-methyl-1,3-propanediyl ester (9CI) (CA INDEX NAME)

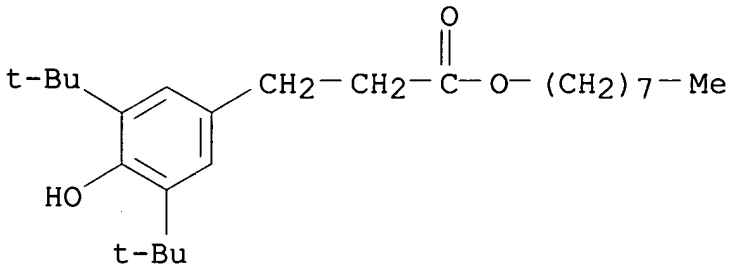
PAGE 1-A



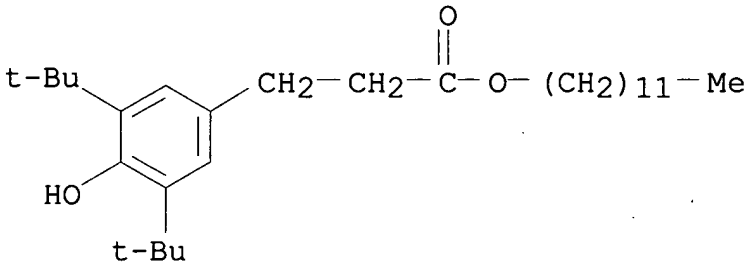
PAGE 1-B

Bu-t

RN 13417-12-4 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octyl ester (9CI) (CA INDEX NAME)

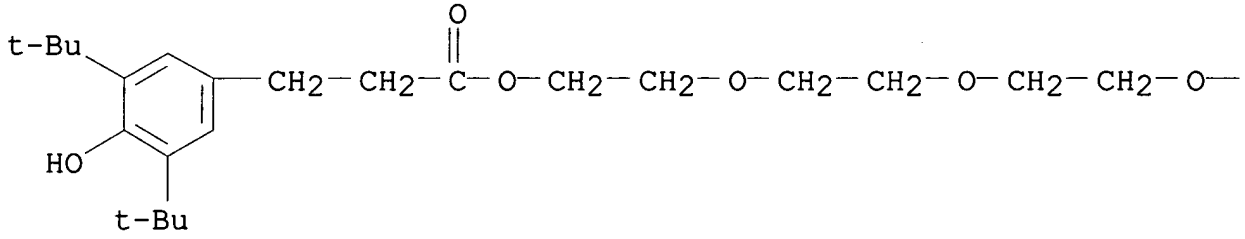


RN 15229-61-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, dodecyl ester (9CI) (CA INDEX NAME)

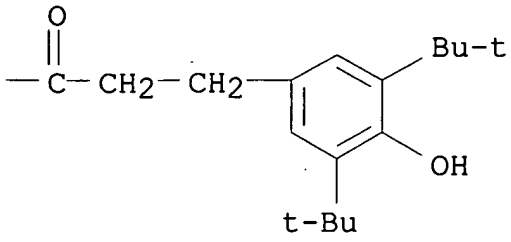


RN 34569-49-8 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester (9CI) (CA INDEX NAME)

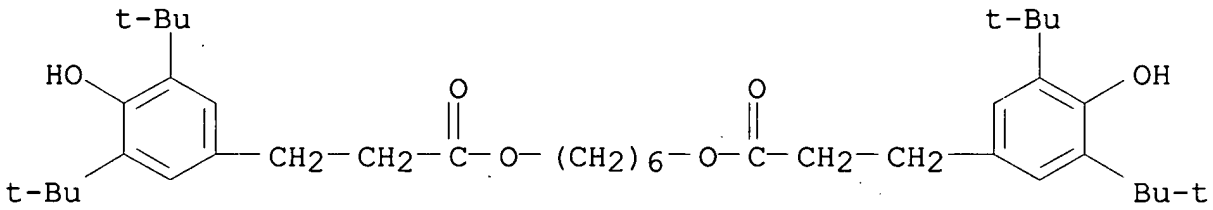
PAGE 1-A



PAGE 1-B

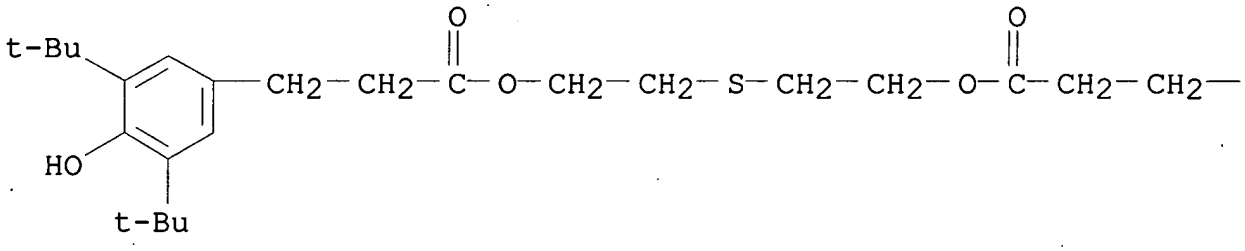


RN 35074-77-2 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)

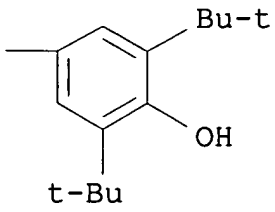


RN 41484-35-9 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

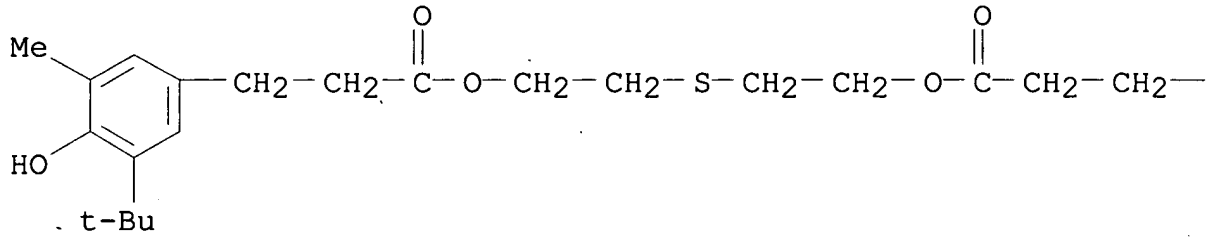


PAGE 1-B

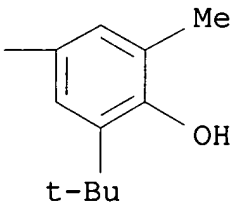


RN 53926-93-5 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

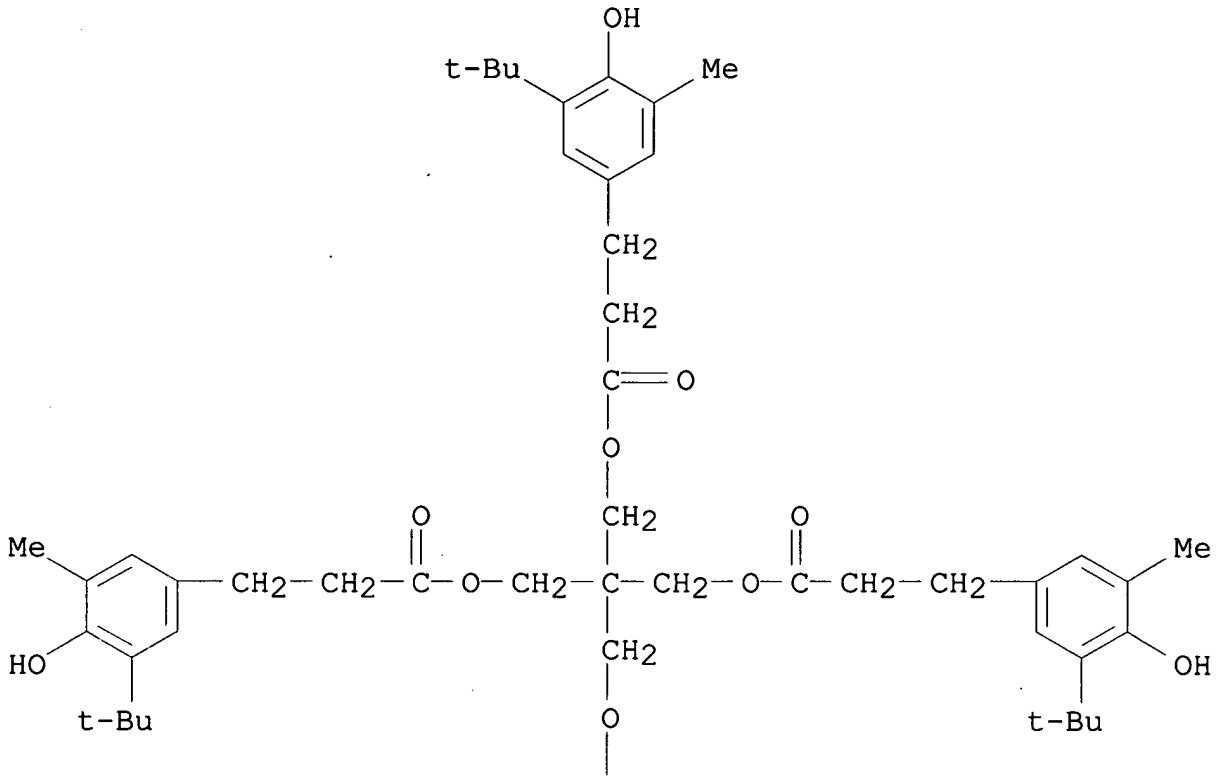


PAGE 1-B

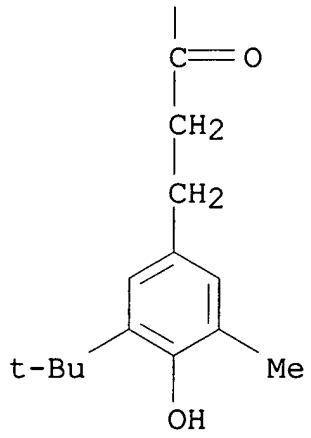


RN 85278-90-6 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, 2,2-bis[[3-[3-(1,1-dimethylethyl)-4-hydroxy-5-methylphenyl]-1-oxopropoxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

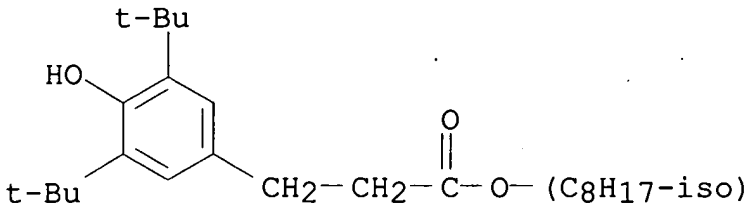


PAGE 2-A

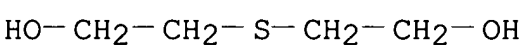


RN 146598-26-7 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-,

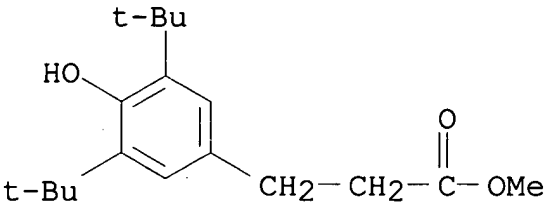
isooctyl ester (9CI) (CA INDEX NAME)



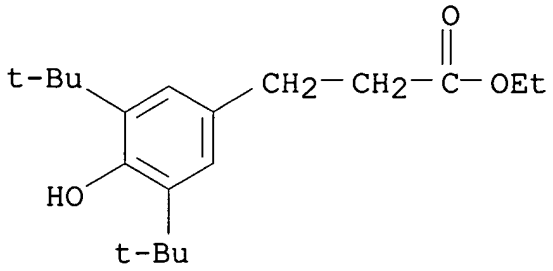
IT **111-48-8**, 2,2'-Thiodiethanol **6386-38-5**, Methyl 3,5-di-tert-butyl-4-hydroxyhydrocinnamate **36294-24-3**, Ethyl 3,5-di-tert-butyl-4-hydroxyhydrocinnamate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(process for the preparation of substituted hydroxyhydrocinnamate esters)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 6386-38-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

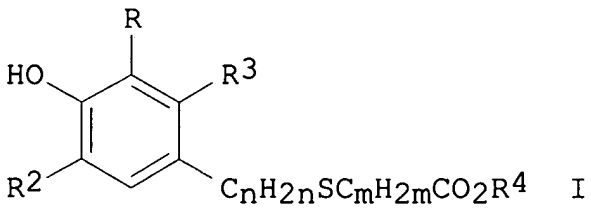


RN 36294-24-3 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



IC ICM C07C069-76
NCL 560075000
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 25, 67
IT **2082-79-3P**, n-Octadecyl 3,5-di-tert-butyl-4-hydroxyhydrocinnamate **6386-68-1P 6683-19-8P 6997-02-0P 13417-12-4P 15229-61-5P 34569-49-8P 35074-77-2P 41484-35-9P 53926-93-5P 85278-90-6P 146598-26-7P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(process for the preparation of substituted hydroxyhydrocinnamate esters)
IT 77-85-0 77-99-6 **111-48-8**, 2,2'-Thiodiethanol 111-87-5, n-Octyl **alcohol**, reactions 112-27-6, Triethylene glycol 112-53-8, Lauryl **alcohol** 112-92-5, n-Octadecyl **alcohol** 115-77-5, Pentaerythritol, reactions 629-11-8, Hexamethylene glycol **6386-38-5**, Methyl 3,5-di-tert-butyl-4-hydroxyhydrocinnamate 26952-21-6, Isooctanol **36294-24-3**, Ethyl 3,5-di-tert-butyl-4-hydroxyhydrocinnamate
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(process for the preparation of substituted hydroxyhydrocinnamate esters)

L48 ANSWER 9 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1998:771375 Document No. 130:27089 Concentrates for use as antioxidants and antiwear additives for fuels, polymer blends, and lubricating oils. Dubs, Paul; Martin, Roger; Evans, Samuel (Ciba Specialty Chemicals Holding Inc., Switz.). Ger. Offen. DE 19822251 A1 19981126, 54 pp. (German). CODEN: GWXXBX.
APPLICATION: DE 1998-19822251 19980518. PRIORITY: EP 1997-810308 19970520.
GI



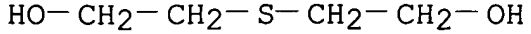
I

AB Concs. for use as antioxidants in fuels (especially gasoline and diesel fuels), polymer blends, and lubricants, are prepared by reaction of components of three structures: (1) an active hydrogen compound, (2) a glyceride; (3) a phenol derivative, and (4) a compound of general formula I [R, R2 = C1-18-alkyl, C2-12-cycloalkyl, Ph, C7-9-phenylalkyl, CnH2n-S-CmH2m-CO2-R4 or -CHRB-S-RA (RA = C4-12-alkyl or Ph; RB = H or Ph); R3 = H, Me, or -CnH2n-S-CmH2m-CO2-R4; R4 = H or C1-8-alkyl; n - 0-2, m = 1-2]. Suitable active hydrogen compds. include pentaerythritol, thiodiethylene glycol, 1,4-butanediol, 1,2-propanediol, diethylene glycol, triethylene glycol, diethanolamine, and glycerin; suitable glycerides include sunflower oil, coconut oil, rapeseed oil, corn oil, safflower oil, castor oil, olive oil, or peanut oil.

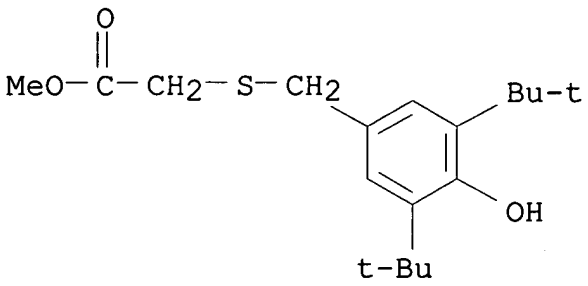
IT **111-48-8DP**, Thiodiethylene glycol, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters **51511-20-7DP**, Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]thio]-, methyl ester, reaction products with glycerides and glycerin **98854-53-6DP**, reaction products with formaldehyde, thioglycolic acid Me ester, glycerin, and rapeseed oil **189880-15-7DP**, Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methyl]thio]-, methyl ester, reaction products with glycerides and glycerin **189880-26-0DP**, Acetic acid, [[(2-hydroxy-3,5-dimethylphenyl)methyl]thio]-, methyl ester, reaction products with glycerides and glycerin **216451-29-5DP**, reaction products with glycerides and glycerin **216451-30-8DP**, reaction products with glycerides and glycerin
RL: MOA (Modifier or additive use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(concs. for use as antioxidants and antiwear additives for fuels, polymer blends, and lubricating oils)

RN 111-48-8 HCAPLUS

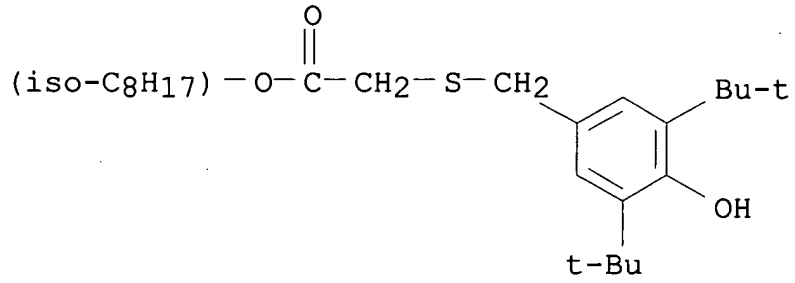
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



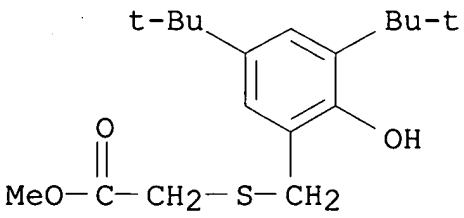
RN 51511-20-7 HCAPLUS
CN Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]thio]-, methyl ester (9CI) (CA INDEX NAME)



RN 98854-53-6 HCAPLUS
CN Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]thio]-, isooctyl ester (9CI) (CA INDEX NAME)

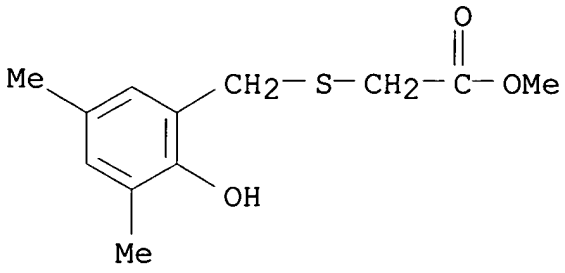


RN 189880-15-7 HCAPLUS
CN Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

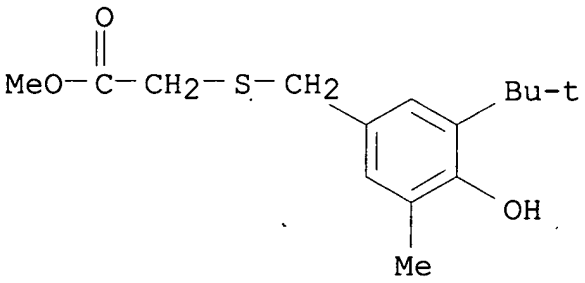


RN 189880-26-0 HCAPLUS

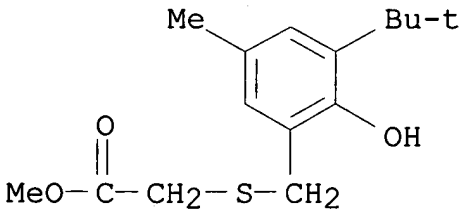
CN Acetic acid, [[(2-hydroxy-3,5-dimethylphenyl)methyl]thio]-, methyl ester (9CI) (CA INDEX NAME)



RN 216451-29-5 HCAPLUS
CN Acetic acid, [[[3-(1,1-dimethylethyl)-4-hydroxy-5-methylphenyl]methyl]thio]-, methyl ester (9CI) (CA INDEX NAME)



RN 216451-30-8 HCAPLUS
CN Acetic acid, [[[3-(1,1-dimethylethyl)-2-hydroxy-5-methylphenyl]methyl]thio]-, methyl ester (9CI) (CA INDEX NAME)



IC ICM C07C323-52
ICS C07H013-04; C07F009-09; C09K015-12; C09K015-28; C10M135-26; C08K005-375; C10L001-14; C07D211-56
ICA C07D249-18; C07D277-70; C07D285-125; C07D493-04
CC 51-8 (Fossil Fuels, Derivatives, and Related Products)
IT 50-00-0DP, Formaldehyde, reaction products with

3,5-di-tert-butylphenol, thioglycolic acid Me ester, glycerin, and rapeseed oil, uses 56-81-5DP, Glycerin, reaction products with glycerides and (hydroxy)benzylthio)acetic acid Me esters 57-55-6DP, 1,2-Propanediol, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters, uses 95-14-7DP, 1H-Benzotriazole, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters 110-63-4DP, 1,4-Butanediol, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters, uses 111-42-2DP, Diethanolamine, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters 111-46-6DP, Diethylene glycol, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters **111-48-8DP**, Thiodiethylene glycol, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters 112-27-6DP, Triethylene glycol, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters 115-77-5DP, Pentaerythritol, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters 1072-71-5DP, 1,3,4-Thiadiazolidine-2,5-dithione, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters 1138-52-9DP, 3,5-Di-tert-butylphenol, reaction products with formaldehyde, thioglycolic acid Me ester, glycerin, and rapeseed oil 2365-48-2DP, Thioglycolic acid methyl ester, reaction products with 3,5-di-tert-butylphenol, formaldehyde, glycerin, and rapeseed oil 26952-21-6DP, Exxal 8, reaction products with 3,5-di-tert-butylphenol, formaldehyde, glycerin, and rapeseed oil 29385-43-1DP, 1H-Benzotriazole, methyl-, reaction products with glycerides, glycerin, and (hydroxy)benzylthioacetic acid esters **51511-20-7DP**, Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]thio]-, methyl ester, reaction products with glycerides and glycerin **98854-53-6DP**, reaction products with formaldehyde, thioglycolic acid Me ester, glycerin, and rapeseed oil **189880-15-7DP**, Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-2-hydroxyphenyl]methyl]thio]-, methyl ester, reaction products with glycerides and glycerin **189880-26-0DP**, Acetic acid, [[(2-hydroxy-3,5-dimethylphenyl)methyl]thio]-, methyl ester, reaction products with glycerides and glycerin **216451-29-5DP**, reaction products with glycerides and glycerin **216451-30-8DP**, reaction products with glycerides and glycerin
RL: MOA (Modifier or additive use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(concs. for use as antioxidants and antiwear additives for fuels, polymer blends, and lubricating oils)

L48 ANSWER 10 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN

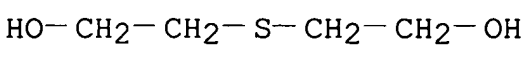
1998:762071 Document No. 130:15685 liquid additive packages containing multifunctional additives for liquid fuels, lubricants, and polymer formulations. Dubs, Paul; Martin, Roger; Boss, Roland; Evans, Samuel (Ciba Specialty Chemicals Holding, Inc., Switz.). Ger. Offen. DE 19820994 A1 19981119, 52 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1998-19820994 19980511. PRIORITY: CH 1997-1123 19970513.

AB Liquid multifunctional additives, especially for use in fuels, lubricants, and polymer formulations, consist of the reaction product of components, consisting of: (1) an active-hydrogen-containing compound, (2) a glyceride or glyceridic oil, (3) a hydroxy-substituted phenylcarboxylic acid, (4) a hydrocarbon oil solvent (typically C9-13-alkylbenzene or C12-20-alkane), and, optionally, a C1-18-alkyl (alkyl)acrylate ester. The active-hydrogen-containing component is suitably chosen from pentaerythritol, thiodiethylene glycol, 1,4-butanediol, 1,2-propanediol, diethylene glycol, triethylene glycol, diethanolamine, or glycerin. Typical glyceridic oils are coconut oil, rape oil, sunflower oil, soybean oil, or castor oil. Component (3) is typically 3-(3'-tert-butyl-4'-hydroxy-5'-methylphenyl)propanoic acid Me ester, 3-(3',5'-di-tert-butyl-4'-hydroxyphenyl)propanoic acid Me ester, and Ar-CH2SCH2CO2Me (Ar = 3,5-di-tert-butyl-4-hydroxyphenyl). The additives esp. have antiwear, antioxidant, and stabilizer (i.e., against heat, light, and oxygen) activity in liq. fuels, lubricating oils, hydraulic fluids, metalworking oils, and polyolefin or polystyrene copolymers.

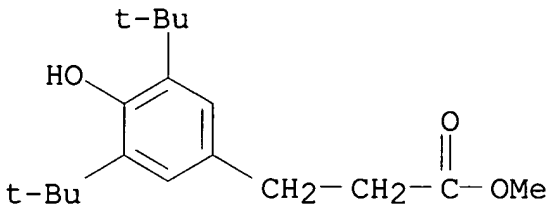
IT **111-48-8D**, Thiodiethylene glycol, reaction products with glycerin and fats and glyceridic oils **6386-38-5D**, Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester, reaction products with glycerin and fats and glyceridic oils **24794-55-6**, Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl- **51511-20-7D**, Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]thio]-, methyl ester, reaction products with glycerin and fats and glyceridic oils
RL: MOA (Modifier or additive use); RCT (Reactant); **RACT (Reactant or reagent)**; USES (Uses)
(additive package containing; packages containing liquid multifunctional additives for liquid fuels, lubricants, and polymers)

RN 111-48-8 HCAPLUS

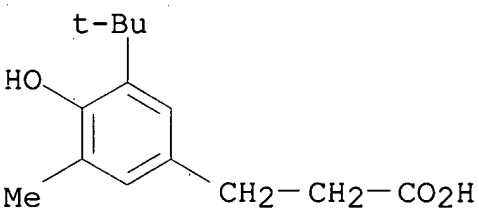
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



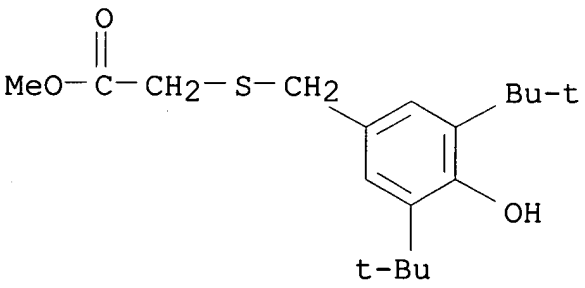
RN 6386-38-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



RN 24794-55-6 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl- (9CI) (CA INDEX NAME)



RN 51511-20-7 HCAPLUS
CN Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]thio]-, methyl ester (9CI) (CA INDEX NAME)



IC ICM C07C069-732
ICS C07C069-54; C07C323-52; C07C229-00; C10M129-74; C10M135-22; C10M133-02; C08K005-00; C10L001-10
ICA C07D211-10; C07D227-00; C07D493-04
CC 51-8 (Fossil Fuels, Derivatives, and Related Products)
IT 56-81-5D, Glycerin, reaction products with fats and glyceridic oils and (di-tertbutyl-hydroxyphenyl)propionic acid Me ester

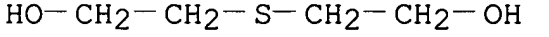
57-55-6D, 1,2-Propanediol, reaction products with glycerin and fats and glyceridic oils, uses 96-33-3D, Methyl acrylate, reaction products with fats and glyceridic oils and (di-tertbutyl-hydroxyphenyl)propionic acid Me ester 110-63-4D, 1,4-Butanediol, reaction products with glycerin and fats and glyceridic oils, uses 111-42-2D, Diethanolamine, reaction products with glycerin and fats and glyceridic oils 111-46-6D, Diethylene glycol, reaction products with glycerin and fats and glyceridic oils **111-48-8D**, Thiodiethylene glycol, reaction products with glycerin and fats and glyceridic oils 112-27-6D, Triethylene glycol, reaction products with glycerin and fats and glyceridic oils 115-77-5D, Pentaerythritol, reaction products with glycerin and fats and glyceridic oils 128-39-2D, 2,6-Di-tert-butylphenol, reaction products with fats and glyceridic oils and (di-tertbutyl-hydroxyphenyl)propionic acid Me ester 2219-82-1D, 2-tert-Butyl-6-methylphenol, reaction products with fats and glyceridic oils and (di-tertbutyl-hydroxyphenyl)propionic acid Me ester **6386-38-5D**, Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester, reaction products with glycerin and fats and glyceridic oils **24794-55-6**, Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl- **51511-20-7D**, Acetic acid, [[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]thio]-, methyl ester, reaction products with glycerin and fats and glyceridic oils
RL: MOA (Modifier or additive use); RCT (Reactant); **RACT (Reactant or reagent)**; USES (Uses)
(additive package containing; packages containing liquid multifunctional
additives for liquid fuels, lubricants, and polymers)

L48 ANSWER 11 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1995:538512 Document No. 122:265035 Liquid antioxidants as stabilizers. Evans, Samuel; Dubs, Paul; Camenzind, Hugo (Ciba-Geigy A.-G., Switz.). Eur. Pat. Appl. EP 644195 A1 19950322, 60 pp. DESIGNATED STATES: R: BE, CH, DE, ES, FR, GB, IT, LI, NL. (German). CODEN: EPXXDW. APPLICATION: EP 1994-810528 19940913. PRIORITY: CH 1993-2844 19930920.
AB The title antioxidants are reaction products from 4 components: (1) a selected diol or analog, such as pentaerythritol, diethanolamine, or glycerin; (2) a triglyceride-type compound such as sunflower or coconut oil; (3) a phenol-containing ester of specified structure; and (4) a compound/element such as diisopropyl dithiophosphate or sulfur. The compds. are useful for stabilizing polymers and lubricants. For example, a mixture of approx. 50 mmol sunflower oil, 50 mmol glycerin, and 0.20 mmol dibutyltin oxide was treated under N at 180-185° with 100 mmol Me 3-(3,5-di-tert-butyl-4-hydroxy)propionate and 0.20 mmol dibutyltin

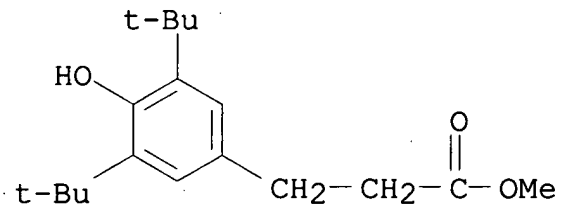
oxide, and after 8 h the mixture was cooled to 100°, treated with 150 mmol sulfur, heated to 180-190°, and cooled, to give a dark, oily product (I) (99%) containing 6.24% sulfur. In the deposit and oxidation panel test, I at 0.6 weight% in a standard lubricating oil reduced deposition from 72 mg to 38 mg. In a similar wear test at 1.0 weight%, I reduced wear scar diameter from 0.91 mm (control) to 0.35 mm.

IT **111-48-8**, Thiodiethylene glycol **6386-38-5**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reactant; preparation of liquid antioxidants as stabilizers for lubricants and polymers)

RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 6386-38-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



IC ICM C07G017-00
ICS C07B045-00; C07C069-732; C07F009-165; C09K015-14; C09K015-08; C09K015-32; C08K005-36; C08K005-134; C08K005-5398

CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 37

IT 56-81-5, Glycerin, reactions 107-56-2 **111-48-8**, Thiodiethylene glycol **6386-38-5** 7704-34-9, Sulfur, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reactant; preparation of liquid antioxidants as stabilizers for lubricants and polymers)

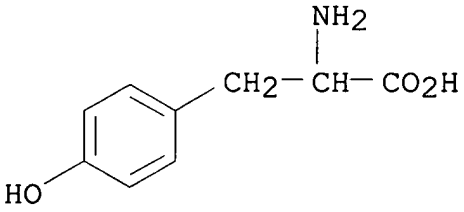
L48 ANSWER 12 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1994:152081 Document No. 120:152081 Collection of enantiomeric

separation factors obtained by capillary gas chromatography on chiral stationary phases. Koenig, W. A. (Univ. Hamburg, Germany). Journal of High Resolution Chromatography, 16(10), 569-86 (English) 1993. CODEN: JHRCE7. ISSN: 0935-6304.

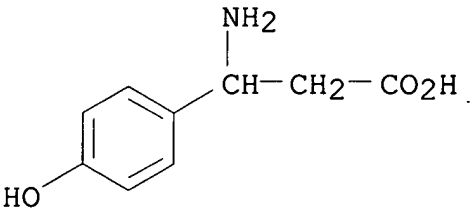
AB Capillary gas chromatog. enantiomeric separation factors, column length, and temperature are tabulated for 295 racemates on the chiral stationary phase octakis(3-O-butyryl-2,6-di-O-pentyl)-γ-cyclodextrin (Lipodex E). The major classes of compds. included: **alcs.**, ketones, carboxylic acids, lactones, hydroxy carboxylic acids, amino acids, and sulfoxides. The racemates were chromatographed either in underivatized form, trifluoroacetates or acetates (many **alcs.**), Me or Et esters (many carboxylic acids), N-trifluoroacetyl derivs. (amino acids), N-alkoxycarbonyl derivs. (histidine), or containing a combination of these derivatizing groups.

IT **556-03-6**, DL-Tyrosine **6049-54-3** **152723-06-3**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(resolution of, by capillary gas chromatog. on chiral cyclodextrin derivative)

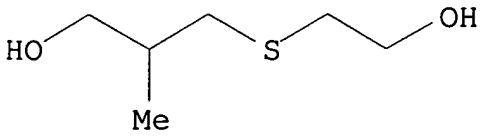
RN 556-03-6 HCAPLUS
CN Tyrosine (9CI) (CA INDEX NAME)



RN 6049-54-3 HCAPLUS
CN Benzenepropanoic acid, β-amino-4-hydroxy- (9CI) (CA INDEX NAME)



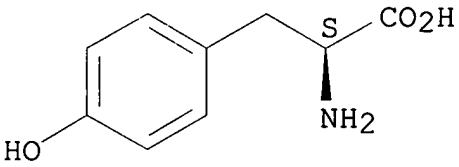
RN 152723-06-3 HCAPLUS
CN 1-Propanol, 3-[(2-hydroxyethyl)thio]-2-methyl- (9CI) (CA INDEX NAME)



IT **60-18-4**, L-Tyrosine, analysis **555-30-6**
556-02-5, D-Tyrosine **2799-15-7**
73025-68-0 152723-07-4 152723-08-5
152786-27-1
RL: PROC (Process)
(separation of, from enantiomer by capillary gas chromatog. on chiral cyclodextrin derivative)

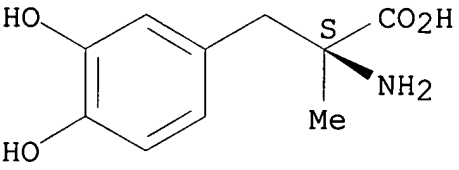
RN 60-18-4 HCAPLUS
CN L-Tyrosine (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



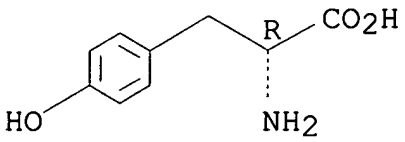
RN 555-30-6 HCAPLUS
CN L-Tyrosine, 3-hydroxy-α-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



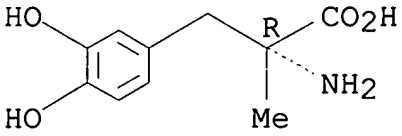
RN 556-02-5 HCAPLUS
CN D-Tyrosine (9CI) (CA INDEX NAME)

Absolute stereochemistry.



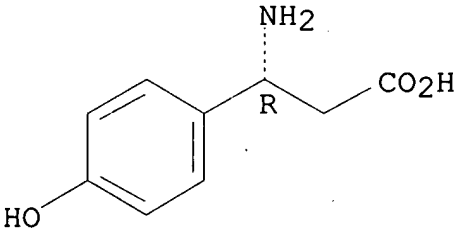
RN 2799-15-7 HCAPLUS
CN D-Tyrosine, 3-hydroxy-α-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



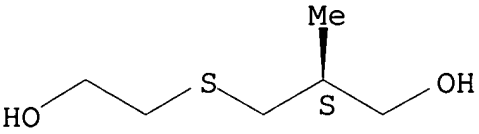
RN 73025-68-0 HCAPLUS
CN Benzenepropanoic acid, β-amino-4-hydroxy-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



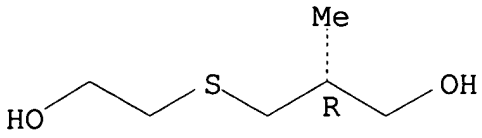
RN 152723-07-4 HCAPLUS
CN 1-Propanol, 3-[(2-hydroxyethyl)thio]-2-methyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



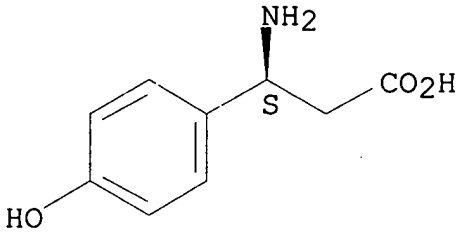
RN 152723-08-5 HCAPLUS
CN 1-Propanol, 3-[(2-hydroxyethyl)thio]-2-methyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 152786-27-1 HCAPLUS
CN Benzenepropanoic acid, β-amino-4-hydroxy-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 78-4 (Inorganic Chemicals and Reactions)
IT **Alcohols**, analysis
Amino acids, analysis
Carboxylic acids, analysis
Ketones, analysis
Lactones
Sulfoxides
RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(resolution of, by capillary gas chromatog. on chiral cyclodextrin derivative)
IT **Alcohols**, analysis
RL: PUR (Purification or recovery); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(carboxy, resolution of, by capillary gas chromatog. on chiral cyclodextrin derivative)
IT 50-12-4, (±)-Mesantoin 54-12-6, DL-Tryptophan 56-82-6, (±)-Glyceraldehyde 57-55-6, (±)-1,2-Propanediol, analysis 59-51-8, DL-Methionine 70-54-2, DL-Lysine 76-22-2, (±)-Camphor 77-41-8, (±)-Mesuximide 78-70-6, (±)-Linalool 78-76-2, (±)-2-Bromobutane 78-92-2, (±)-2-Butanol 80-57-9, (±)-Verbenone 80-58-0, (±)-2-Bromobutanoic acid 80-68-2, DL-Threonine 86-34-0, (±)-Phensuximide 86-35-1, (±)-Ethotoin 89-78-1,

(±)-Menthol 89-80-5, (±)-Menthone 89-81-6,
(±)-Piperitone 90-64-2, (±)-Mandelic acid 93-54-9,
(±)-1-Phenyl-1-propanol 93-56-1, (±)-Phenyl-1,2-ethanediol
93-72-1 94-65-5, (±)-2-Propylcyclohexanone 96-09-3
96-20-8, (±)-2-Amino-1-butanol 98-55-5, (±)-α-
Terpineol 98-85-1, (±)-1-Phenylethanol 99-49-0,
(±)-Carvone 104-50-7 105-21-5 106-22-9,
(±)-β-Citronellol 106-69-4, (±)-1,2,6-Hexanetriol
107-81-3, (±)-2-Bromopentane 107-88-0, (±)-1,3-Butanediol
108-11-2, (±)-4-Methyl-2-pentanol 108-29-2,
(±)-4-Methylbutyrolactone 115-95-7, (±)-Linalyl acetate
116-53-0, (±)-2-Methylbutanoic acid 123-96-6,
(±)-2-Octanol 124-76-5, (±)-Isoborneol 127-91-3,
(±)-β-Pinene 144-90-1, DL-3-Amino-2-methylpropanoic acid
144-98-9, DL-Allo-threonine 150-30-1, DL-Phenylalanine
302-72-7, DL-Alanine 302-84-1, DL-Serine 319-84-6 328-39-2,
DL-Leucine 340-05-6, (±)-1-Phenyl-2,2,2-trifluoroethanol
443-79-8, DL-Isoleucine 471-84-1, (±)-α-Fenchene
472-46-8, (±)-cis-α-Irone 491-07-6, (±)-Isomenthone
496-67-3, (±)-Bromisoval 498-21-5, (±)-Methylsuccinic acid
507-70-0, (±)-Borneol 513-86-0, (±)-Acetoin 515-00-4,
(±)-Myrtenol 515-94-6, DL-2,3-Diaminopropanoic acid
516-06-3, DL-Valine 535-75-1, DL-Pipecolic acid 536-50-5
541-48-0, DL-3-Aminobutanoic acid 541-85-5, (±)-5-Methyl-3-
heptanone 543-49-7, (±)-2-Heptanol 547-64-8, (±)-Methyl
lactate 552-63-6, (±)-Tropic acid **556-03-6**,
DL-Tyrosine 556-52-5, (±)-2,3-Epoxy-1-propanol 557-35-7,
(±)-2-Bromooctane 562-74-3, (±)-Terpinen-4-ol 564-94-3,
(±)-Myrtenal 565-74-2, (±)-2-Bromo-3-methylbutanoic acid
583-60-8, (±)-2-Methylcyclohexanone 584-03-2,
(±)-1,2-Butanediol 584-93-0, (±)-2-Bromopentanoic acid
589-82-2, (±)-3-Heptanol 589-98-0, (±)-3-Octanol
591-11-7, (±)-Angelicalactone 595-39-1, DL-Isovaline
597-44-4, (±)-Citramalic acid 598-72-1, (±)-2-
Bromopropanoic acid 598-78-7, (±)-2-Chloropropanoic acid
599-45-1, (±)-trans-α-Irone 600-15-7,
(±)-2-Hydroxybutanoic acid 614-19-7 616-05-7,
(±)-2-Bromohexanoic acid 616-07-9, DL-Ornithine 616-30-8,
(±)-3-Amino-1,2-dihydroxypropane 617-45-8, DL-Aspartic acid
617-65-2, DL-Glutamic acid 617-73-2, (±)-2-Hydroxyoctanoic
acid 618-28-0 618-36-0, (±)-1-Phenylethylamine 626-93-7,
(±)-2-Hexanol 636-48-6, (±)-Ethylsuccinic acid 642-92-2
696-75-3 698-76-0 698-87-3, (±)-1-Phenyl-2-propanol
705-86-2 706-14-9 710-04-3 713-95-1 765-42-4 766-43-8
823-22-3 938-97-6 1074-33-5 1077-28-7 1114-07-4
1124-13-6 1134-47-0, DL-Baclofen 1193-82-4, (±)-Methyl
phenyl sulfoxide 1195-79-5, (±)-Fenchone 1436-34-6,
(±)-1,2-Epoxyhexane 1438-14-8, (±)-Isopropyloxirane

1460-57-7, (±)-trans-1,2-Cyclohexanediol 1461-97-8
1524-12-5, (±)-1-Phenylethyl trifluoroacetate 1569-60-4,
(±)-6-Methyl-5-hepten-2-ol 1669-98-3, (±)-Ethyl methyl
sulfoxide 1674-08-4, (±)-trans-Pinocarveol 1674-30-2,
(±)-2-Chloro-1-phenylethanol 1713-33-3 1740-84-7
1893-99-8, (±)-3-Octyl trifluoroacetate 1974-04-5,
(±)-2-Bromoheptane 2088-07-5, (±)-2-Methyl-1-penten-3-ol
2109-22-0, (±)-2-Cyclohexylpropanal 2305-32-0 2382-59-4,
(±)-2-Methyl-3-oxobutanoic acid 2507-55-3,
(±)-2-Hydroxytetradecanoic acid 2566-33-8, DL-N-Methylleucine
2835-81-6, DL-2-Aminobutanoic acid 2933-94-0, (±)-Toliprolol
2976-98-9, (±)-Butyl methyl sulfoxide 2984-55-6,
(±)-2-Hydroxydodecanoic acid 3107-04-8, DL-Allo-isoleucine
3301-90-4 3301-94-8 3319-15-1, (±)-1-(4-Methoxyphenyl)-1-
ethanol 3374-22-9, DL-Cysteine 3377-86-4, (±)-2-Bromohexane
3391-86-4, (±)-1-Octen-3-ol 3395-35-5, DL-3,4-Dehydroproline
3506-26-1 4170-24-5, (±)-2-Chlorobutanoic acid 4170-69-8,
(±)-Isopropyl phenyl sulfoxide 4294-45-5 4423-94-3,
(±)-2-Ethylcyclohexanone 5343-92-0, (±)-1,2-Pentanediol
5424-29-3, DL-2-Methylserine 5895-35-2 6032-29-7,
(±)-2-Pentanol **6049-54-3** 6137-11-7,
(±)-4-Methyl-3-heptanone 6168-72-5 6351-10-6,
(±)-1-Indanol 6532-76-9 6915-15-7, (±)-Malic acid
6982-25-8, (±)-2,3-Butanediol 7124-40-5, (±)-1,2-
Cyclooctadiene 7287-81-2 7370-92-5 7493-90-5 7519-74-6,
(±)-Thiocamphor 10397-68-9, (±)-N,N-Dimethyl-2-
chloropropanamide 13136-04-4 13838-16-9, (±)-Enflurane
14292-26-3, (±)-3-Hydroxydecanoic acid 14292-27-4,
(±)-3-Hydroxyoctanoic acid 14314-21-7, (±)-Ipsenol
14375-45-2, (±)-Abscisic acid 14575-74-7 15358-88-0,
(±)-Isopinocamphone 15573-40-7 15677-15-3 15932-80-6,
(±)-Pulegone 16194-32-4, (±)-trans-Pityol 16423-19-1,
(±)-Geosmin 16485-10-2 17042-16-9, (±)-4-Methyl-3-
hexanone 17417-00-4 18952-34-6, (±)-trans-1,3-
Cycloheptanediol 19362-93-7 19362-95-9 19362-96-0
20182-77-8 20894-95-5, (±)-1-Oxo-1-furanyl-2-propanol
22083-74-5, (±)-Nicotine 22554-74-1, (±)-trans-3,4-
Dihydroxytetrahydrofuran 23355-97-7 23433-07-0,
(±)-1,3-Nonanediol 26287-61-6 26287-62-7, DL-2-Methylvaline
26675-46-7, (±)-Isoflurane 29094-05-1 29602-28-6
29674-47-3, (±)-Methyl 2-hydroxybutanoate 30820-22-5,
(±)-Grandisol 33105-81-6, DL-Tert-leucine 34199-35-4
36402-52-5, (±)-2,4-Pentanediol 37442-40-3 37666-84-5
39638-67-0 41708-72-9, DL-Tocainide 42565-22-0,
(±)-trans-1,2-Cyclooctanediol 49761-17-3 50471-44-8,
(±)-Vinclozoline 52153-41-0 52940-41-7,
(±)-1,2-Diaminopentane 53771-14-5 54814-61-8,
(±)-6-Hexyl-3-methoxy-5,6-dihydro-2-pyranone 55013-32-6

59042-49-8 59042-50-1 60018-04-4, (±)-exo-Brevicomin
60212-41-1, (±)-trans-2-Ethoxycyclopropanecarboxylic acid
60478-96-8, (±)-Frontalin 61274-28-0 62532-53-0,
(±)-endo-Brevicomin 63493-28-7, (±)-2-Aminopentane
64577-18-0, (±)-trans-1,4-Cyclooctanediol 65899-13-0,
(±)-3-Methylnonanal 68756-64-9, (±)-Methyl
2-hydroxyhexanoate 71666-04-1, (±)-cis-2-
Ethoxycyclopropanecarboxylic acid 77772-07-7,
(±)-3-Methyldecanal 78019-28-0 78086-85-8 78087-36-2,
(±)-Lineatin 81308-06-7 81655-41-6 82373-92-0
100507-95-7, (±)-1-Methyl-trans-1,3-cyclohexanediol
101325-32-0, (±)-cis-γ-Irone 107597-39-7,
(±)-cis-Pityol
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(resolution of, by capillary gas chromatog. on chiral cyclodextrin derivative)

IT 108740-82-5, (±)-Methyl 2-hydroxypentanoate 113349-34-1
113786-52-0, (±)-2-Chloro-3-(octyloxy)propanoic acid
122674-44-6, (±)-trans-1,2-Cyclodecanediol 125284-13-1
128535-00-2 128707-59-5 128821-87-4, (±)-Phaseic acid
134359-16-3 137144-03-7, (±)-7-Methoxymethyl-1,7-dimethyl-
1,3,5-cycloheptatriene 137144-04-8, (±)-7-Methoxymethyl-2,7-
dimethyl-1,3,5-cycloheptatriene 137144-17-3 138664-39-8
139132-44-8 140631-52-3 144299-82-1 148323-45-9
148323-48-2 151297-46-0 152212-14-1, (±)-2-Oxo-1-
pentylcyclohexanecarboxylic acid 152212-15-2,
(±)-1-Methyl-2-oxocyclohexanecarboxylic acid 152722-57-1
152722-60-6 152722-63-9 152722-66-2 152722-71-9
152722-74-2 152722-77-5 152722-80-0 152722-83-3
152722-86-6 152722-89-9 152722-91-3 152722-97-9
152723-06-3 152723-33-6 152723-36-9,
(±)-1-(2-Cyanoethyl)-2-oxocyclohexanecarboxylic acid
152723-41-6 152723-50-7 152723-55-2 152723-61-0
152723-67-6, (±)-Methyl 2-chloro-3-(benzyloxy)propanoate
152723-70-1, (±)-Ethyl 2-chloro-3-(benzyloxy)propanoate
152723-73-4 152723-76-7 152723-77-8 152723-78-9
152786-07-7 152786-08-8 152786-09-9 153061-60-0
156304-56-2
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(resolution of, by capillary gas chromatog. on chiral cyclodextrin derivative)

IT 51-35-4 52-90-4, L-Cysteine, analysis 54-11-5, (-)-Nicotine
56-41-7, L-Alanine, analysis 56-45-1, L-Serine, analysis
56-84-8, L-Aspartic acid, analysis 56-86-0, L-Glutamic acid,
analysis 56-87-1, L-Lysine, analysis **60-18-4**,
L-Tyrosine, analysis 61-90-5, L-Leucine, analysis 63-68-3,
L-Methionine, analysis 63-91-2, L-Phenylalanine, analysis
70-26-8, L-Ornithine 72-18-4, L-Valine, analysis 72-19-5,

L-Threonine, analysis 73-22-3, L-Tryptophan, analysis 73-32-5, L-Isoleucine, analysis 81-13-0 87-69-4, analysis 89-82-7, (+)-Pulegone 97-67-6, (-)-Malic acid 126-90-9, (+)-Linalool 126-91-0, (-)-Linalool 147-71-7 153-94-6, D-Tryptophan 312-84-5, D-Serine 319-78-8, D-Isoleucine 328-38-1, D-Leucine 338-69-2, D-Alanine 340-06-7, (+)-1-Phenyl-2,2,2-trifluoroethanol 348-66-3, D-Ornithine 348-67-4, D-Methionine 453-17-8, (+)-Glyceraldehyde 464-43-7, (+)-Borneol 464-45-9, (-)-Borneol 464-48-2, (-)-Camphor 464-49-3, (+)-Camphor 473-62-1, (+)-Isopinocamphone 473-85-8 497-09-6, (-)-Glyceraldehyde 512-13-0 547-61-5, (-)-trans-Pinocarveol **555-30-6 556-02-5**, D-Tyrosine 595-40-4, L-Isovaline 611-71-2, (-)-Mandelic acid 613-87-6, (-)-1-Phenyl-1-propanol 618-27-9 632-20-2, D-Threonine 636-61-3, (+)-Malic acid 640-68-6, D-Valine 673-06-3, D-Phenylalanine 687-28-5, (-)-Ethylsuccinic acid 697-64-3, (-)-1-Indanol 715-58-2 763-95-1, (+)-Butyl methyl sulfoxide 921-01-7, D-Cysteine 923-27-3, D-Lysine 1072-86-2, (-)-trans-1,2-Cyclohexanediol 1077-27-6 1117-61-9, (+)-β-Citronellol 1190-94-9 1191-24-8, (+)-2-Bromooctane 1196-01-6, (-)-Verbenone 1196-31-2, (+)-Isomenthone 1200-22-2 1445-91-6, (-)-1-Phenylethanol 1492-24-6, L-2-Aminobutanoic acid 1509-34-8, L-Allo-isoleucine 1509-35-9, D-Allo-isoleucine 1517-68-6, (+)-1-Phenyl-2-propanol 1517-69-7, (+)-1-Phenylethanol 1517-70-0 1565-74-8, (+)-1-Phenyl-1-propanol 1572-95-8, (-)-1-Phenyl-2-propanol 1572-97-0 1701-82-2 1723-00-8, D-Pipecolic acid 1730-91-2, (+)-2-Methylbutanoic acid 1783-96-6, D-Aspartic acid 1915-96-4, D-2,3-Diaminopropanoic acid 2140-95-6, D-3-Amino-2-methylpropanoic acid 2174-58-5, (-)-Methylsuccinic acid 2216-51-5, (-)-Menthol 2217-02-9, (+)-Fenchol 2244-16-8, (+)-Carvone 2319-57-5 2418-52-2 2438-10-0, (+)-Terpinen-4-ol 2584-71-6 2623-91-8, D-2-Aminobutanoic acid 2627-86-3, (-)-1-Phenylethylamine 2681-94-9 2749-11-3, (+)-Alaninol **2799-15-7** 2825-91-4 3059-97-0, D-Isovaline 3060-46-6, L-N-Methylleucine 3105-95-1, L-Pipecolic acid 3275-37-4 3347-90-8, (+)-2-Hydroxybutanoic acid 3391-87-5, (+)-Menthone 3391-90-0, (-)-Pulegone 3398-22-9 3641-51-8, (+)-Methylsuccinic acid 3687-48-7, (-)-1-Octen-3-ol 3775-72-2, L-3-Aminobutanoic acid 3775-73-3, D-3-Aminobutanoic acid 3886-69-9, (+)-1-Phenylethylamine 3966-58-3 4033-39-0, L-2,3-Diaminopropanoic acid 4043-88-3, L-3,4-Dehydroproline 4074-24-2, (+)-Ethylsuccinic acid 4198-87-2, (-)-Toliprolol 4198-88-3, (+)-Toliprolol 4221-99-2, (+)-2-Butanol 4249-19-8, L-3-Amino-2-methylpropanoic acid 4254-14-2, (-)-1,2-Propanediol, analysis 4254-15-3, (+)-1,2-Propanediol, analysis 4518-66-5 4573-50-6, (-)-Piperitone 4695-62-9, (+)-Fenchone 4850-71-9, (+)-Methyl

phenyl sulfoxide 5753-30-0 5787-32-6, (+)-2-Bromobutane 5787-33-7, (-)-2-Bromobutane 5856-62-2, (+)-2-Amino-1-butanol 5856-63-3, (-)-2-Amino-1-butanol 5978-55-2, (-)-2-Bromooctane 5978-70-1, (-)-2-Octanol 6033-23-4, (+)-2-Heptanol 6033-24-5, (-)-2-Heptanol 6061-13-8 6091-50-5, (+)-Piperitone 6169-06-8, (+)-2-Octanol 6236-09-5, (+)-Citramalic acid 6236-10-8, (-)-Citramalic acid 6290-03-5, (-)-1,3-Butanediol 6485-40-1, (-)-Carvone 6516-09-2 6712-78-3, (+)-Myrtenol 6893-26-1, D-Glutamic acid 7298-96-6 7298-98-8 7298-99-9 7378-37-2, (-)-α-Fenchene 7474-05-7, (+)-2-Chloropropanoic acid 7540-51-4, (-)-β-Citronellol 7785-53-7, (+)-α-Terpineol 7787-20-4, (-)-Fenchone 10009-70-8, (+)-2-Bromopropanoic acid 10334-13-1, (-)-Isoborneol 10482-56-1, (-)-α-Terpineol 10531-50-7, (-)-1-Phenyl-2,2,2-trifluoroethanol 13921-90-9 14073-97-3, (-)-Menthone 14212-54-5 14398-53-9, (-)-Abscisic acid 14575-93-0 14590-54-6 14898-79-4, (-)-2-Butanol 14898-80-7, (+)-4-Methyl-2-pentanol 15356-60-2, (+)-Menthol 16202-15-6, (-)-Tropic acid 16320-13-1 16355-00-3, (-)-Phenyl-1,2-ethanediol 16404-54-9, (-)-4-Methyl-2-pentanol 16417-36-0 16509-46-9, (-)-Linalyl acetate 16725-71-6, (+)-Isoborneol 16820-18-1, L-2-Methylserine 17126-67-9, (+)-Tropic acid 17199-29-0, (+)-Mandelic acid 17224-72-5 17224-73-6 17257-71-5 17392-83-5, (+)-Methyl lactate 18172-67-3, (-)-β-Pinene 18309-28-9, (-)-Isomenthone 18309-32-5, (+)-Verbenone 18453-46-8, (-)-Methyl phenyl sulfoxide 18486-69-6, (-)-Myrtenal 18899-29-1 18899-31-5 19041-15-7, (-)-4-Methylbutyrolactone 19132-06-0, (+)-2,3-Butanediol 19525-80-5 19526-23-9 19700-21-1, (-)-Geosmin 19894-97-4, (-)-Myrtenol 19894-98-5, (+)-trans-Pinocarveol 19902-08-0, (+)-β-Pinene 20016-85-7, (-)-2-Hydroxybutanoic acid 20086-34-4, (+)-4-Methyl-3-hexanone 20126-76-5, (-)-Terpinen-4-ol 20290-99-7, (+)-exo-Brevicomin 20445-31-2 20480-40-4, (+)-trans-1,2-Cyclooctanediol 20580-77-2, (-)-Ethyl methyl sulfoxide 20616-93-7, (+)-5-Methyl-3-heptanone 20710-33-2 20710-34-3 20780-53-4 20780-54-5 20859-02-3, L-Tert-leucine 21293-29-8, (+)-Abscisic acid 21917-20-4 21963-41-7, (+)-Cyclohexane-trans-1,2-dicarboxylic acid 22194-21-4, (+)-Enflurane 22194-22-5, (-)-Enflurane 22554-27-4, (+)-2-Methylcyclohexanone 22554-29-6, (-)-2-Methylcyclohexanone 22617-19-2, (-)-2-Ethylcyclohexanone 22625-19-0, (+)-endo-Brevicomin 22658-92-0, (+)-3-Octanol 22818-40-2 23727-16-4, (+)-Myrtenal 24347-58-8, (-)-2,3-Butanediol 24347-63-5 24394-14-7, (-)-Phaseic acid 24587-53-9, (+)-1-Octen-3-ol 24621-61-2, (+)-1,3-Butanediol 24629-25-2 24830-94-2, D-Allo-threonine 25162-00-9, (+)-Nicotine 25501-32-0, (+)-1-Indanol 25779-13-9, (+)-Phenyl-1,2-ethanediol 26184-62-3, (-)-2-Pentanol

26451-15-0, (+)-Ethyl methyl sulfoxide 26532-22-9, (+)-Grandisol
26549-24-6, (-)-2-Hexanol 26549-25-7, (+)-3-Heptanol
26632-17-7 26782-71-8, D-Tert-leucine 26782-75-2 27109-48-4
27109-49-5 27871-49-4, (-)-Methyl lactate 28379-57-9,
(+)-Hydroxydanaidal 28379-58-0, (-)-Hydroxydanaidal
RL: PROC (Process)
(separation of, from enantiomer by capillary gas chromatog. on chiral cyclodextrin derivative)

IT 28387-15-7, (+)-2-Hydroxydodecanoic acid 28401-39-0,
(-)-Frontalin 28941-54-0, (+)-2-Bromohexane 28954-12-3,
L-Allo-threonine 29117-44-0, (-)-2-Bromopentane 29117-54-2,
(-)-1,2-Pentanediol 29587-89-1 29617-66-1,
(-)-2-Chloropropanoic acid 29882-58-4, (+)-2-Bromopentane
30117-44-3 30365-50-5 31087-44-2, (+)-2-Pentanol 31321-74-1,
D-N-Methylleucine 31323-51-0 32231-50-8, (-)-2-Methylbutanoic
acid 32462-30-9 32644-15-8, (-)-2-Bromopropanoic acid
32653-32-0, (-)-2-Chlorobutanoic acid 32659-49-7 32835-74-8
33796-86-0 33985-20-5, (-)-2-Aminopentane 34044-66-1,
(+)-Isopropyl phenyl sulfoxide 34202-45-4 35124-13-1,
(+)-cis-α-Irone 35124-14-2, (-)-trans-α-Irone
35124-16-4, (+)-cis-γ-Irone 35320-23-1, (-)-Alaninol
35628-05-8, (-)-Ipsenol 36302-45-1, (-)-2-Propylcyclohexanone
39122-22-0 39122-23-1 40348-66-1, (-)-1,2-Butanediol
40521-06-0 40856-44-8 41807-37-8, (-)-Ethotoin 42070-91-7
42070-92-8 42075-32-1, (-)-2,4-Pentanediol 42990-12-5
43112-32-9 44987-72-6 46022-05-3 50987-15-0 51096-08-3
51154-53-1 51154-54-2 51532-30-0, (+)-4-Methyl-3-heptanone
51532-31-1, (-)-4-Methyl-3-heptanone 51685-40-6, (+)-Linalyl
acetate 51795-48-3, (-)-Butyl methyl sulfoxide 52019-78-0,
(+)-2-Hexanol 52078-93-0, (+)-Thiocamphor 53402-10-1,
(-)-Thiocamphor 53584-56-8, (-)-Acetoin 53940-82-2,
D-2-Methylvaline 53940-83-3 53984-26-2 53984-75-1
54053-45-1, (+)-2-Chlorobutanoic acid 54542-13-1,
(+)-2-Aminopentane 55123-01-8 55637-37-1 55667-40-8
55701-03-6 55701-08-1 55701-09-2 56246-59-4 56246-60-7
56751-12-3, (-)-2-Chloro-1-phenylethanol 56936-59-5 56936-66-4
57044-25-4, (+)-2,3-Epoxy-1-propanol 57287-27-1 57794-08-8,
(+)-trans-1,2-Cyclohexanediol 57917-96-1, (+)-Frontalin
58287-20-0 58616-97-0 58640-72-5, D-3,4-Dehydroproline
58917-25-2, (+)-4-Methylbutyrolactone 58917-26-3,
(+)-6-Methyl-5-hepten-2-ol 58917-27-4, (-)-6-Methyl-5-hepten-2-
ol 58958-05-7, (+)-Ipsenol 59285-67-5 60456-23-7,
(-)-2,3-Epoxy-1-propanol 61278-21-5 62322-48-9 62393-67-3
62393-68-4 62701-49-9, (-)-3-Heptanol 62885-28-3,
(-)-2-Bromohexane 63357-96-0 63357-97-1 64313-75-3,
(-)-exo-Brevicomin 64440-09-1 65035-34-9, (+)-Lineatin
66211-46-9 66514-99-6, L-Baclofen 67113-13-7,
(+)-2-Propylcyclohexanone 67253-09-2 68225-45-6, (-)-Grandisol

69308-37-8, D-Baclofen 70111-05-6, (+)-2-Chloro-1-phenylethanol
70267-25-3, (-)-2-Hydroxydodecanoic acid 70267-27-5
70492-66-9, (-)-3-Octanol 70989-04-7, (+)-Mesantoin
71140-51-7, (-)-Mesantoin 72155-50-1 72345-23-4,
(+)-2,4-Pentanediol **73025-68-0** 73349-07-2 73349-08-3
73522-17-5, (+)-1,2-Butanediol 73649-91-9, (-)-Lineatin
73992-47-9, (+)-7-Methoxymethyl-2,7-dimethyl-1,3,5-
cycloheptatriene 73992-48-0, (-)-7-Methoxymethyl-2,7-dimethyl-
1,3,5-cycloheptatriene 73992-49-1, (+)-7-Methoxymethyl-1,7-
dimethyl-1,3,5-cycloheptatriene 74561-18-5 75599-12-1,
(+)-2-Ethylcyclohexanone 75880-65-8 76652-86-3 76652-88-5
76792-22-8 77858-08-3, (-)-4-Methyl-3-hexanone 77882-09-8
78183-56-9, (+)-Acetoin 80041-00-5 80041-01-6 80225-50-9,
(-)-Isopropyl phenyl sulfoxide 80952-67-6, (-)-endo-Brevicomin
81083-99-0 81132-44-7, D-2-Methylserine 82378-47-0
84709-85-3 84953-52-6 86562-29-0 88270-38-6 88593-95-7,
(+)-N,N-Dimethyl-2-chloropropanamide 88996-94-5 89888-03-9,
(-)-cis-α-Irone 89888-04-0, (-)-cis-γ-Irone
90242-81-2, (+)-trans-α-Irone 90244-32-9 91423-83-5
91423-84-6 92694-51-4 92806-43-4 95912-79-1 96488-07-2
97233-03-9 97233-04-0 97673-81-9 97949-70-7 98168-21-9,
(-)-2-Methyl-1-penten-3-ol 98672-68-5 99461-66-2 99461-67-3
104873-46-3, (+)-Geosmin 104898-06-8, (+)-1,2-Epoxyhexane
105015-53-0 105119-22-0 105814-93-5 105814-94-6
106225-85-8 107797-24-0 107797-25-1 107797-26-2
107797-27-3 107983-40-4 108268-29-7, (-)-trans-1,2-
Cyclooctanediol 108340-61-0, (+)-1,2-Pentanediol 108739-43-1,
(+)-Ethotoin 108812-74-4 108861-12-7 108861-13-8
108936-10-3, (-)-N,N-Dimethyl-2-chloropropanamide 108943-43-7
108943-44-8 108943-45-9 108943-46-0 108943-47-1
109061-96-3 109785-15-1 110916-84-2 111321-36-9
114179-07-6 116003-10-2, (-)-5-Methyl-3-heptanone 116724-26-6,
(+)-α-Fenchene 118025-93-7, (+)-trans-1,3-Cycloheptanediol
118025-94-8, (-)-trans-1,3-Cycloheptanediol 119911-69-2
119911-70-5 121541-59-1 121541-65-9 121570-10-3
122517-46-8 124330-64-9 125637-07-2, (+)-2-Methyl-1-penten-3-
ol 126935-12-4 126935-13-5 127062-02-6 127516-44-3,
(+)-Phaseic acid 130232-55-2, (+)-1,2,6-Hexanetriol
130232-56-3, (-)-1,2,6-Hexanetriol 130232-91-6,
(+)-2-Bromoheptane 130232-92-7, (-)-2-Bromoheptane
130404-08-9, (-)-1,2-Epoxyhexane 133098-04-1 133098-05-2
135672-61-6 135672-62-7 136377-93-0 138597-08-7
138597-09-8 138597-10-1 138597-15-6 138597-16-7
138597-17-8 138597-18-9 138810-04-5 142896-75-1
143724-87-2, (-)-6-Hexyl-3-methoxy-5,6-dihydro-2-pyranone
144370-25-2 144370-26-3 144370-27-4 144370-29-6
144370-30-9 144370-31-0 144370-32-1 144370-33-2
148323-50-6 148323-51-7 148323-52-8 148323-54-0

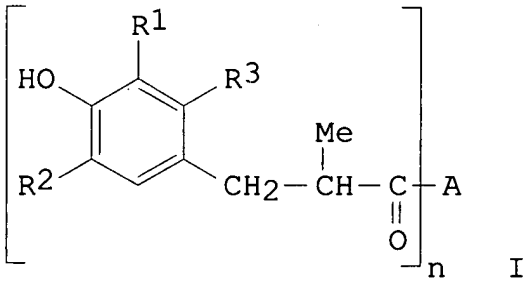
148323-55-1 148323-57-3 152212-37-8, (+)-2-Oxo-1-pentylcyclohexanecarboxylic acid 152212-38-9, (+)-1-Methyl-2-oxocyclohexanecarboxylic acid 152212-50-5
RL: PROC (Process)
(separation of, from enantiomer by capillary gas chromatog. on chiral cyclodextrin derivative)

IT 152212-61-8, (-)-2-Oxo-1-pentylcyclohexanecarboxylic acid 152212-62-9, (-)-1-Methyl-2-oxocyclohexanecarboxylic acid 152212-74-3 152722-58-2 152722-59-3 152722-61-7 152722-62-8 152722-64-0 152722-65-1 152722-67-3 152722-68-4 152722-69-5 152722-70-8 152722-72-0 152722-73-1 152722-75-3 152722-76-4 152722-78-6 152722-79-7 152722-81-1 152722-82-2 152722-84-4 152722-85-5 152722-87-7 152722-88-8 152722-90-2 152722-92-4 152722-93-5 152722-95-7, (+)-3-Octyl trifluoroacetate 152722-96-8, (-)-3-Octyl trifluoroacetate 152722-98-0 152722-99-1 152723-01-8, (+)-1-Methyl-trans-1,3-cyclohexanediol 152723-02-9, (-)-1-Methyl-trans-1,3-cyclohexanediol 152723-04-1, (+)-trans-1,4-Cyclooctanediol 152723-05-2, (-)-trans-1,4-Cyclooctanediol **152723-07-4** **152723-08-5** 152723-09-6, (-)-7-Methoxymethyl-1,7-dimethyl-1,3,5-cycloheptatriene 152723-10-9 152723-11-0 152723-13-2 152723-14-3 152723-16-5, (+)-3-Methylnonanal 152723-17-6, (-)-3-Methylnonanal 152723-19-8, (+)-3-Methyldecanal 152723-20-1, (-)-3-Methyldecanal 152723-21-2 152723-22-3 152723-24-5, (+)-1-Oxo-1-furanyl-2-propanol 152723-25-6, (-)-1-Oxo-1-furanyl-2-propanol 152723-28-9, (+)-trans-2-Ethoxycyclopropanecarboxylic acid 152723-29-0, (-)-trans-2-Ethoxycyclopropanecarboxylic acid 152723-31-4, (+)-cis-2-Ethoxycyclopropanecarboxylic acid 152723-32-5, (-)-cis-2-Ethoxycyclopropanecarboxylic acid 152723-34-7 152723-35-8 152723-37-0, (+)-1-(2-Cyanoethyl)-2-oxocyclohexanecarboxylic acid 152723-38-1, (-)-1-(2-Cyanoethyl)-2-oxocyclohexanecarboxylic acid 152723-39-2 152723-40-5 152723-42-7 152723-43-8 152723-45-0, (+)-1,2-Diaminopentane 152723-46-1, (-)-1,2-Diaminopentane 152723-48-3 152723-49-4 152723-51-8 152723-52-9 152723-53-0, (+)-Vinclozoline 152723-54-1, (-)-Vinclozoline 152723-56-3 152723-57-4 152723-59-6 152723-60-9 152723-62-1 152723-63-2 152723-65-4, (+)-2-Chloro-3-(octyloxy)propanoic acid 152723-66-5, (-)-2-Chloro-3-(octyloxy)propanoic acid 152723-68-7, (+)-Methyl 2-chloro-3-(benzyloxy)propanoate 152723-69-8, (-)-Methyl 2-chloro-3-(benzyloxy)propanoate 152723-71-2, (+)-Ethyl 2-chloro-3-(benzyloxy)propanoate 152723-72-3, (-)-Ethyl 2-chloro-3-(benzyloxy)propanoate 152723-74-5 152723-75-6 152723-79-0 152723-80-3 152786-10-2 152786-11-3 152786-12-4, (+)-trans-1,2-Cyclodecanediol 152786-13-5, (-)-trans-1,2-Cyclodecanediol

152786-20-4 152786-21-5 152786-23-7 152786-24-8
152786-25-9 **152786-27-1** 152786-28-2 152786-30-6
152786-31-7 152786-32-8 152786-33-9 153061-61-1
153061-62-2, (+)-6-Hexyl-3-methoxy-5,6-dihydro-2-pyranone
160895-35-2 160895-36-3
RL: PROC (Process)
(separation of, from enantiomer by capillary gas chromatog. on chiral cyclodextrin derivative)

L48 ANSWER 13 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1991:491843 Document No. 115:91843 Preparation of (p-hydroxyphenyl)propanoate esters as stabilizers for photographic dyes and couplers. Leppard, David G.; Rody, Jean (Ciba-Geigy A.-G., Switz.). Eur. Pat. Appl. EP 415883 A2 19910306, 43 pp. DESIGNATED STATES: R: DE, FR, GB, IT. (German). CODEN: EPXXDW. APPLICATION: EP 1990-810624 19900820. PRIORITY: CH 1989-3104 19890828.

GI



I

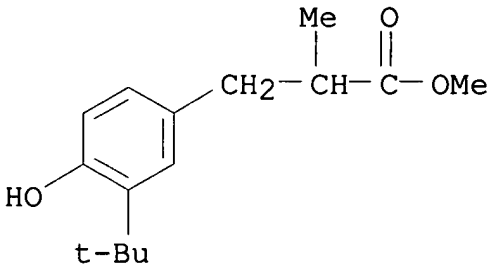
AB The title compds. I [R1 = C1-18 alkyl, (un)substituted C5-12 cycloalkyl, Ph, C7-9 aralkyl; R2 = H, any of definitions for R1; R3 = H, Me; A = OR4, NR5R6, OXO, etc., with provisos; R4 = C1-24 alkyl, C3-23 (un)substituted alkyl optionally interrupted by O, S, NR7; R5, R6 = H, C1-12 alkyl, C3-8 alkenyl, (un)substituted C5-12 cycloalkyl, (un)substituted Ph, etc.; R7 = H, C1-12 alkyl, allyl, PhCH2, etc.; X = C2-10 alkylene, C4-8 alkenylene, cyclohexylene, etc.] were prepared by transesterification of Me (3-tert-butyl- or 3,5-di-tert-butyl-4-hydroxyphenyl)-2-methylpropanoate with the appropriate **alcs**. Thus, 91.9 g Me 2-methyl-3-(3',5'-di-tert-butyl-4'-hydroxyphenyl)propionate and 18.3 g S(CH2CH2OH)2 were heated to 100°, 0.4 g Bu2SnO was added, and the mixture heated 6 h at 180° with removal of MeOH to give 72.4% title compound (I; R1 = R2 = CMe3, R3 = H, A = OCH2CH2SCH2CH2O, n = 2) (II). A photog. emulsion layer (preparation given) containing II had 12%
color d. decrease in a Weather-Ometer test vs. 33% for a control

without stabilizer.

IT **135409-64-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and transesterification of, in preparation of photog. color stabilizers)

RN 135409-64-2 HCAPLUS

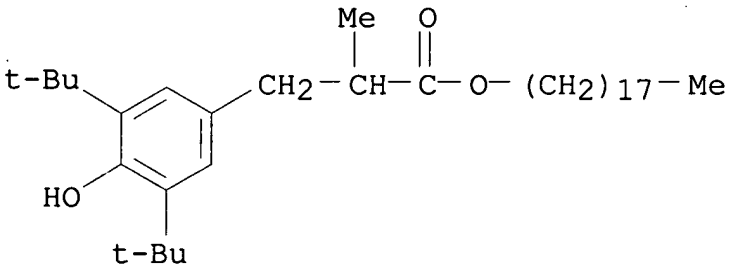
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-α-methyl-, methyl ester (9CI) (CA INDEX NAME)



IT **130183-18-5P 130183-23-2P 135409-61-9P 135409-62-0P 135409-63-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as photog. color stabilizer)

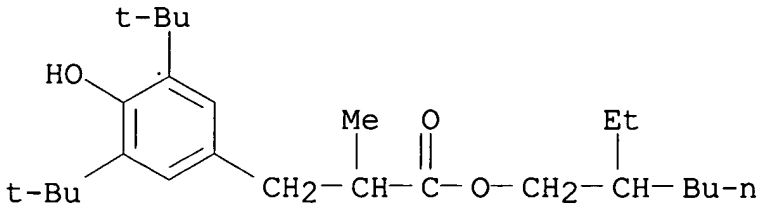
RN 130183-18-5 HCAPLUS

CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-, octadecyl ester (9CI) (CA INDEX NAME)

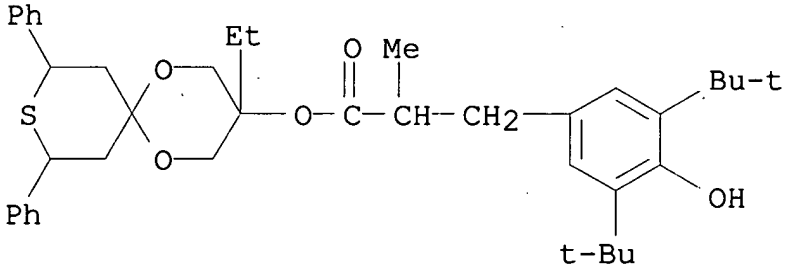


RN 130183-23-2 HCAPLUS

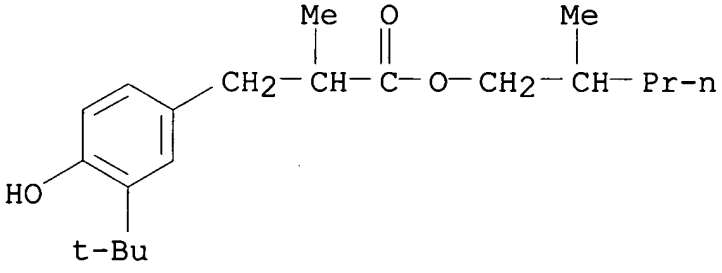
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-, 2-ethylhexyl ester (9CI) (CA INDEX NAME)



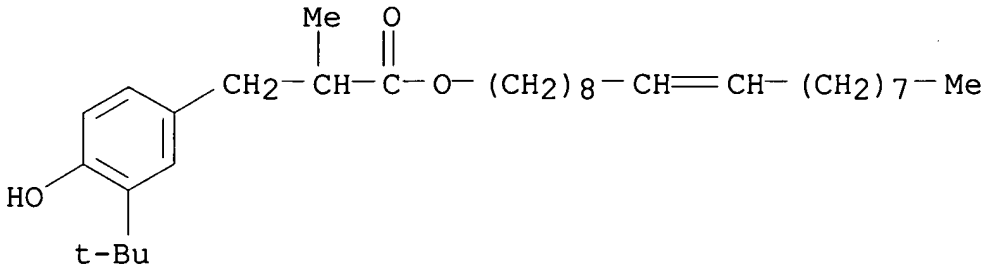
RN 135409-61-9 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-, 3-ethyl-8,10-diphenyl-1,5-dioxa-9-thiaspiro[5.5]undec-3-yl ester (9CI) (CA INDEX NAME)



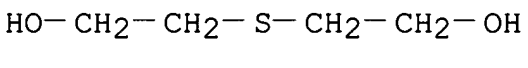
RN 135409-62-0 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-α-methyl-, 2-methylpentyl ester (9CI) (CA INDEX NAME)



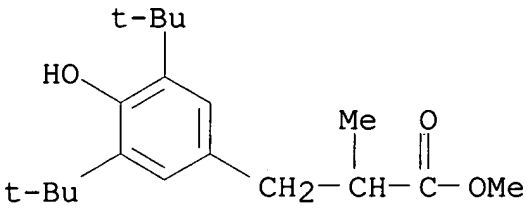
RN 135409-63-1 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-α-methyl-, 9-octadecenyl ester (9CI) (CA INDEX NAME)



IT **111-48-8**, Thiodiethyleneglycol
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(transesterification by, of Me (hydroxyphenyl)propanoate derivative, in preparation of photog. color stabilizer)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



IT **98618-86-1**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(transesterification of, in preparation of photog. color stabilizers)
RN 98618-86-1 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-, methyl ester (9CI) (CA INDEX NAME)



IC ICM G03C007-392
ICS G03C007-388
ICA C07C039-00
CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 74
IT **135409-64-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**

(preparation and transesterification of, in preparation of photog. color stabilizers)

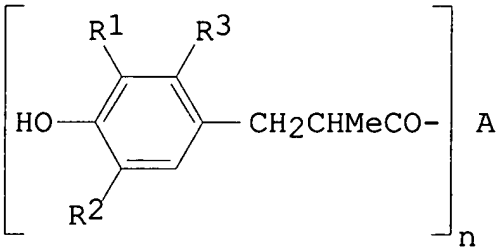
IT **130183-18-5P 130183-23-2P 135409-61-9P 135409-62-0P 135409-63-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as photog. color stabilizer)

IT 104-76-7, 2-Ethyl-1-hexanol 105-30-6, 2-Methyl-1-pentanol **111-48-8**, Thiodiethyleneglycol 112-92-5, 1-Octadecanol 593-47-5, 9-Octadecen-1-ol 135409-65-3
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(transesterification by, of Me (hydroxyphenyl)propanoate derivative, in preparation of photog. color stabilizer)

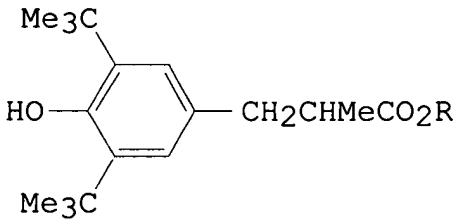
IT **98618-86-1**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(transesterification of, in preparation of photog. color stabilizers)

L48 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1990:611576 Document No. 113:211576 Preparation of (hydroxyphenyl)isobutyrates as antioxidants. Evans, Samuel (Ciba-Geigy A.-G., Switz.). Eur. Pat. Appl. EP 366040 A1 19900502, 81 pp. DESIGNATED STATES: R: BE, CH, DE, ES, FR, GB, IT, LI, NL. (German). CODEN: EPXXDW. APPLICATION: EP 1989-119641 19891023. PRIORITY: CH 1988-3959 19881025.

GI



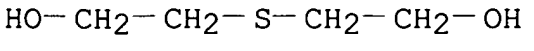
I



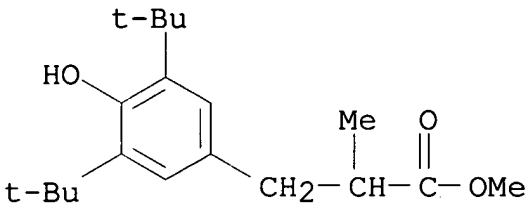
II

AB The title compds. [I; A = alkoxy, (substituted)NH2, tetramethylpiperidyloxy, oxyalkyleneoxy, oxytetramethylpiperidinoethoxy, OCH2CH2N(CH2CH2O)2, OCH(CH2O)2, O[CH2C(CH2O)3]2, etc.; R1, R2 = alkyl, cycloalkyl, Ph, aralkyl; R3 = H, Me; n = 1-4, 6] were prepared Thus, hydroxyphenylisobutyrate II (R = Me) was heated 6 h at 180° with 1-octadecanol and Bu2SnO to give II (R = octadecyl) which gave acid value 0.11 mg KOH/g oil and 22 mg sludge at 0.25 weight% in a lubricating oil in ASTM D 934/DIN 51587/IP 157 oxidation test.

IT **111-48-8 98618-86-1**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reaction of, in preparation of antioxidants)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

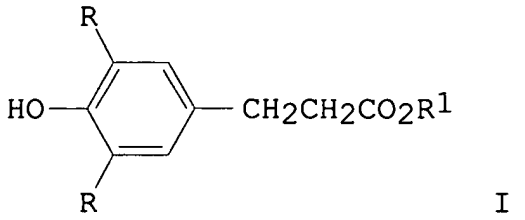


RN 98618-86-1 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-α-methyl-, methyl ester (9CI) (CA INDEX NAME)

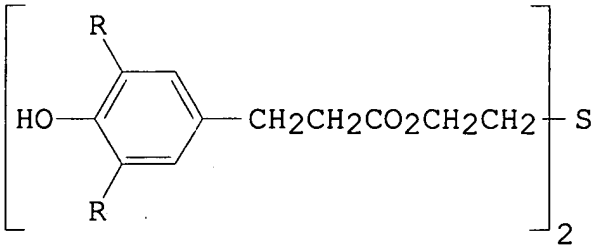


IC ICM C07C069-732
ICS C07C235-34; C08K005-00; C09K015-04; C10M129-76; C10M133-16
CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 102-71-6, reactions 104-76-7 111-46-6, reactions
111-48-8 112-53-8, 1-Dodecanol 112-92-5, 1-Octadecanol
143-08-8, 1-Nonanol 629-11-8, 1,6-Hexanediol 7803-57-8,
Hydrazine hydrate 27458-94-2, Isononylalcohol **98618-86-1**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reaction of, in preparation of antioxidants)

L48 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1986:478668 Document No. 105:78668 Stearyl β-(3,5-dibutyl-4-hydroxyphenyl)propionate and bis[β-(3,5-dibutyl-4-hydroxybenzyl)methylcarboxyethyl] sulfide. Ahlfors, Matts; Koskimies, Salme; Lahtinen, Leila; Idelman, Peter (Neste Oy, Finland). PCT Int. Appl. WO 8600301 A1 19860116, 14 pp. DESIGNATED STATES: W: DK, JP, NO, SU, US; RW: BE, CH, DE, FR, GB, LU, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1985-FI63 19850628. PRIORITY: FI 1984-2618 19840628.
GI



I



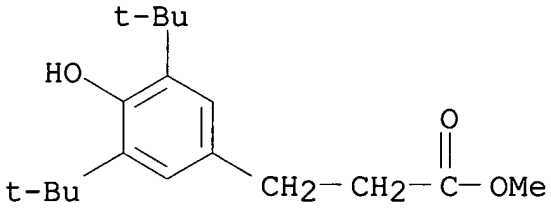
II

AB The title compds. (I and II; R = n-, sec-, iso-, or tert-Bu; R1 = stearyl), useful as stabilizers for rubbers and plastics (no data), are prepared by transesterification of I (R1 = C1-4 alkyl) with stearyl **alc.** or thiodiglycol in the presence of a titanate catalyst. Thus, addition of 2,6-(Me3C)2C6H3OH to CH2:CHCO2Me using Me3COK in Me3COH gave 70% I (R = Me3C, R1 = Me), which (6.0 g) was heated with 5.4 g stearyl **alc.** at 100°/50 mmHg. Tetra-Bu titanate (0.1 mL) was added, the mixture heated 3 h at 95°/5 mmHg with distillation of MeOH, 0.05 mL addnl. catalyst added, and the reaction continued for 30 min and worked up to give 8.5 g (80%) I (R = Me3C, R1 = stearyl). A similar transesterification with thiodiglycol gave 79% II.

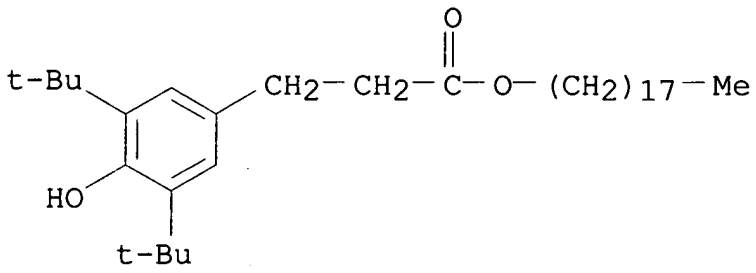
IT **6386-38-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and transesterification of)

RN 6386-38-5 HCAPLUS

CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

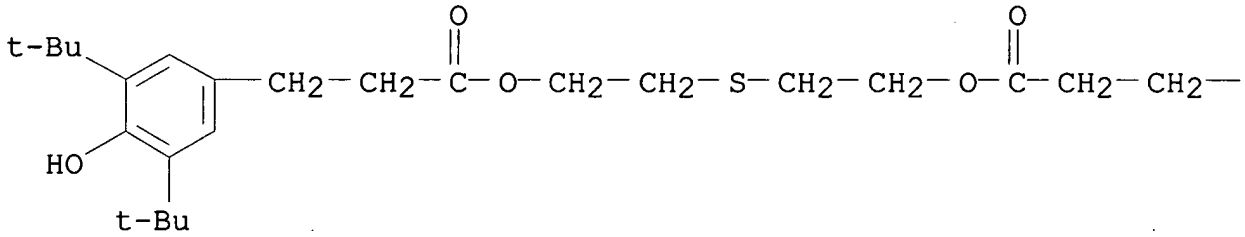


IT **2082-79-3P 41484-35-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by transesterification, titanate catalysts for)
RN 2082-79-3 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (9CI) (CA INDEX NAME)

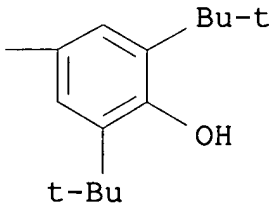


RN 41484-35-9 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

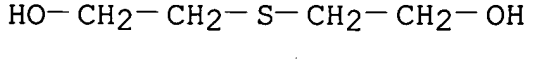


PAGE 1-B



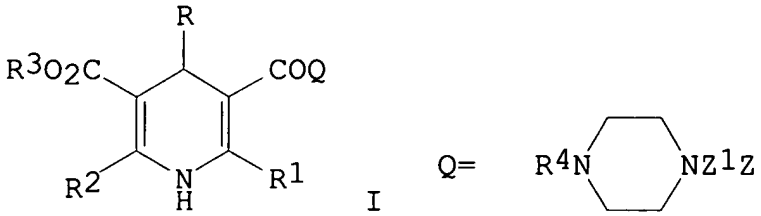
IT **111-48-8**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(transesterification of, with Me di-tert-butylhydroxyphenylpropionate)

RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



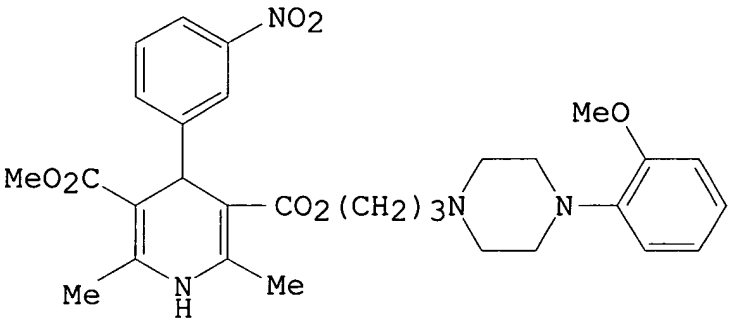
IC ICM C07C069-732
ICS C07C069-76
CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 37, 39
IT **6386-38-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and transesterification of)
IT **2082-79-3P 41484-35-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by transesterification, titanate catalysts for)
IT **111-48-8** 112-92-5
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(transesterification of, with Me di-tert-butylhydroxyphenylpropionate)

L48 ANSWER 16 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1986:88595 Document No. 104:88595 Dihydropyridinyldicarboxylic acid piperazinyl derivatives and a pharmaceutical agent containing them. Poindexter, Graham S.; Temple, Davis L. (Bristol-Myers Co., USA). Ger. Offen. DE 3512995 A1 19851017, 62 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1985-3512995 19850411. PRIORITY: US 1984-599097 19840411; US 1985-693426 19850122.
GI



I

Q=



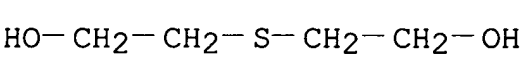
IV

AB The title compds. [I: R = cycloalkyl, bicycloalkenyl, aryl, heteroaryl; R1, R2 = (un)substituted alkyl; R3 = R1, Q; R4 = (un)substituted Ph, pyridinyl, pyrimidinyl; Z = O, NH; Z1 = alkylene, optionally containing O, S, or NH] were prepared Thus, Cl(CH2)3OH was esterified with diketene to give 82% MeCOCH2CO2(CH2)3Cl (II). 3-O2NC6H4CHO was condensed with MeCOCH2CO2Me to give 82% 3-O2NC6H4CH:C(COMe)CO2Me (III). II and III were refluxed in EtOH with NH4OAc to give 99% I [R = 3-O2NC6H4, R1-R3 = Me, Q = Cl(CH2)3O] which was refluxed with 1-(2-methoxyphenyl)piperazine in MeCN containing Et3N and a catalytic amount of KI to give 17% piperazinylpropyl ester IV. IV was equal or superior to nifedipine as a calcium blocker and as an α-adrenergic blocker in standard in vivo and in vitro tests.

IT **111-48-8**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(acetoacetylation of, by diketene)

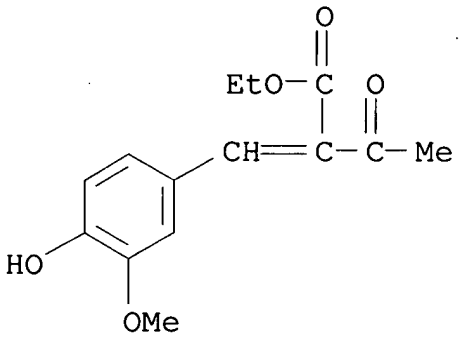
RN 111-48-8 HCAPLUS

CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



IT **89082-79-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and cyclocondensation of, with acetoacetates and

ammonium acetate)
RN 89082-79-1 HCAPLUS
CN Butanoic acid, 2-[(4-hydroxy-3-methoxyphenyl)methylene]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)

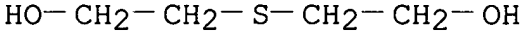


IC ICM C07D401-12
ICS C07D401-14; C07D211-90; C07D295-04; A61K031-495; A61K031-44
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **111-48-8** 627-30-5 34885-02-4 40004-65-7 40255-48-9
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(acetoacetylation of, by diketene)
IT 620-80-4P 5453-80-5P 15725-20-9P 15725-23-2P 17448-84-9P
25315-75-7P 31330-47-9P 39562-16-8P 39562-17-9P
39562-38-4P 54756-29-5P 62760-10-5P 69022-96-4P
89082-76-8P 89082-77-9P 89082-78-0P **89082-79-1P**
102382-09-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and cyclocondensation of, with acetoacetates and ammonium acetate)

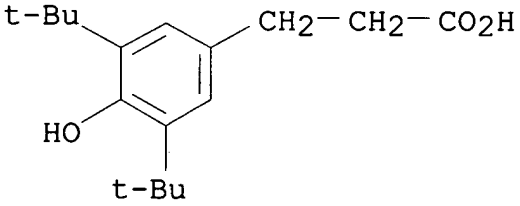
L48 ANSWER 17 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1984:513740 Document No. 101:113740 Boron-containing heterocyclic compounds and lubricating oils containing them. Holstedt, Richard A.; Jessup, Peter; Baron, Kenneth; Croudace, Michael C. (Union Oil Co., USA). PCT Int. Appl. WO 8401169 A1 19840329, 97 pp. DESIGNATED STATES: W: JP; RW: AT, BE, CH, DE, FR, GB, LU, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1983-US1295 19830822. PRIORITY: US 1982-418196 19820915; US 1982-434602 19821015; US 1983-476513 19830318.
AB The preparation and use of B-containing heterocyclic compds. imparting extreme-pressure, antiwear, and friction-reducing properties to lubricating oils are described. The lubricating oil is also provided with a hydrocarbon polysulfide derivative of 2,5-dimercapto-1,3,4-thiadiazole as Cu corrosion inhibitor or

terephthalic acid [100-21-0] as Pb corrosion inhibitor and a diphenylamine derivative oxidation inhibitor. Thus, a B-containing heterocyclic compound was prepared by reacting under reflux 20 g H3BO3 with 95 g Armak Ethomeen C/12 [bis(2-hydroxyethyl)cocoamine] in 250 mL PhMe for 1 h. The product [5-(cocoalkyl)-1-hydroxy-5-aza-1-bova-2,8-dioxacyclooctane] when used in 1 weight% concentration in SAE 10 W/40 oil considerablly reduced the torque on a metal journal as compared to the oil without the additive.

IT **111-48-8**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(esterification of, with (3,5-di-tert-butyl-4-hydroxy)hydrocinnamic acid)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



IT **20170-32-5**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(esterification of, with 2,2-dihydroxydiethyl suflide)
RN 20170-32-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy- (9CI) (CA INDEX NAME)

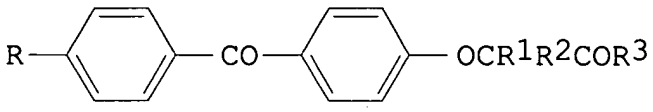


IC C10M001-54; C10M001-38; C07F007-00; C07C107-02; C07G017-00
CC 51-8 (Fossil Fuels, Derivatives, and Related Products)
IT **111-48-8**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(esterification of, with (3,5-di-tert-butyl-4-hydroxy)hydrocinnamic acid)
IT **20170-32-5**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(esterification of, with 2,2-dihydroxydiethyl suflide)

L48 ANSWER 18 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1980:215092 Document No. 92:215092 Benzoylphenoxyalkanoic acid

derivatives and their therapeutic use. (Alfa Farmaceutici S.p.A., Italy). Fr. Demande FR 2425425 19791207, 22 pp. (French). CODEN: FRXXBL. APPLICATION: FR 1979-11587 19790508.

GI



I

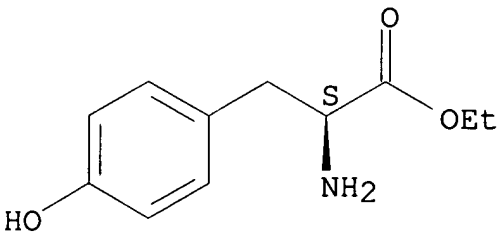
AB α-(4-Benzoylphenoxy)alkanoyl chlorides were amidated and esterified to give I [R = Cl, Br, iodo, alkyl; R1 and R2 (same or different) are H, alkyl, hydroxyalkyl; R3 = OH, alkoxy, NR4CR5R6CO2R7 [R4 = H, alkyl; R5 and R6 (same or different) are H, alkyl, hydroxyalkyl, mercaptoalkyl, alkylaryl, aryl; R7 = H, alkyl], NHCH2CONHCH2CO2H, 2-(nicotinoyloxy)ethylamino, 3-(nicotinoyloxy)propylamine, NHCH2CH2SO3H, OCH2CO2R8 (R8 = H, alkyl), piperidinoamino, (hexamethyleneimino)amino, 2-nicotinoyloxyethoxy, 3-nicotinoyloxypropoxy, 2-nicotinamidoethoxy, (4-ClC6H4OCMe2CO2CH2CH2)2N, [3,4,5-(MeO)3C6H2CO2CH2CH2]2N, bis(2-nicotinoyloxyethyl)amino], which exhibited anticholesteremic activity. The reaction of 4-(4-ClC6H4CO)C6H4OCMe2COCl with H2NCH2CO2H and NaOH gave I (R = Cl, R1 = R2 = Me, R3 = NHCH2CO2H).

IT **949-67-7**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(amidation of phenoxyisobutyryl chloride derivative by)

RN 949-67-7 HCAPLUS

CN L-Tyrosine, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



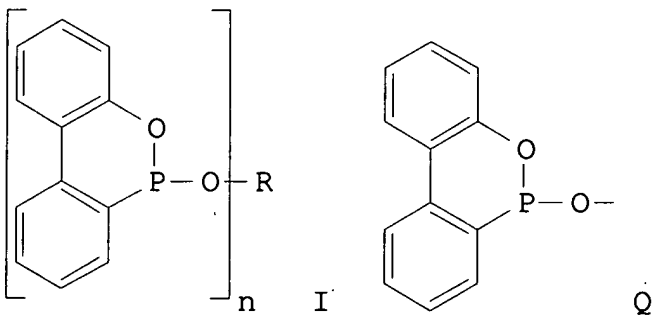
IT **111-48-8**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(esterification of phenoxyisobutyryl chloride derivative by)

RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

HO—CH_2—CH_2—S—CH_2—CH_2—OH

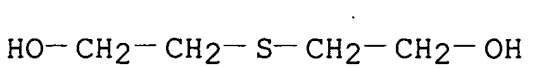
IC C07C103-30; C07C059-25; C07C069-66; C07C093-187
CC 25-19 (Noncondensed Aromatic Compounds)
IT 56-40-6, reactions 107-35-7 111-42-2, reactions 156-87-6
556-50-3 617-27-6 **949-67-7** 2213-43-6 5619-07-8
5680-79-5 5680-80-8 38345-94-7 52605-49-9 72676-16-5
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(amidation of phenoxyisobutyryl chloride derivative by)
IT 105-59-9 **111-48-8** 623-50-7 6265-73-2
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(esterification of phenoxyisobutyryl chloride derivative by)

L48 ANSWER 19 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1980:146908 Document No. 92:146908 Cyclic phosphonite stabilizers.
Rasberger, Michael; Spivack, John D. (Ciba-Geigy Corp., USA).
U.S. US 4185006 19800122, 11 pp. (English). CODEN: USXXAM.
APPLICATION: US 1978-922394 19780706.
GI

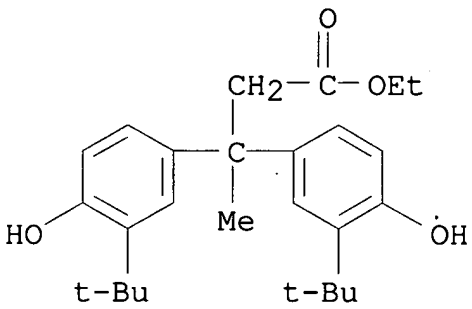


AB Eight title phosphonites I (R = an n-valent aliphatic, alicyclic, aromatic or araliph. which may contain N, O or S or heterocyclics; n = 2-6) were prepared by esterification of 6-chlorodibenz[c,e][1,2]oxaphosphorine (II) with a polyol, Q(OH)n. Thus, 0.1 mol 2,5-di-tert-butylhydroquinone and 0.2 mol II were heated 3 h at 200° to give 2,5-(Me3C)2C6H2Q2-1,4. Similarly prepared were [4,3-Q(Me3C)C6H3]2CMe2, (QCH2)2CMe2 and (QCH2CH2)2S. I were polymer stabilizers, e.g., for polypropylene.

IT **111-48-8 52785-98-5**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reaction of, with chlorodibenzoxaphosphorine)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



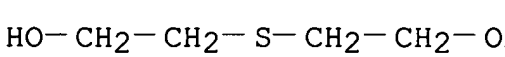
RN 52785-98-5 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-β-[3-(1,1-dimethylethyl)-4-hydroxyphenyl]-4-hydroxy-β-methyl-, ethyl ester (9CI) (CA INDEX NAME)



IC C07F009-48; C07F009-65; C08K005-53
NCL 260045800N
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 36, 37
IT 79-96-9 88-58-4 **111-48-8** 118-82-1 126-30-7
629-11-8 903-19-5 **52785-98-5**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reaction of, with chlorodibenzoxaphosphorine)

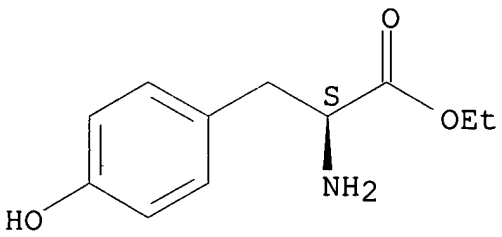
L48 ANSWER 20 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1980:76135 Document No. 92:76135 Benzene phenoxyalkanoic acid derivatives with hypolipemic activity. (Alfa Farmaceutici S.p.A., Italy). Belg. BE 876094 19790903, 27 pp. (French). CODEN: BEXXAL. APPLICATION: BE 1979-57777 19790508.
AB 4-XC6H4COC6H4OCRR1COR2 [I; X = Br, Cl, iodo, alkyl; R, R1 = H, alkyl, hydroxyalkyl; R2 = Q(CH2)nR3, where Q = NH or O, n = 1-3, and R3 = nicotinoyloxy, SO3H, CONHCH2CO2H, piperidinoamino, etc.], which showed hypolipemic activity, were prepared Thus, H2NCH2CO2H treated with 4-ClC6H4COC6H4OCMe2COCl-4 in Et2O-2N NaOH gave I (X = Cl, R = R1 = Me, R2 = NHCH2CO2H) which, at 0.2 mmol/kg, lowered triglycerides in the blood of the rats by 50.7%.

IT **111-48-8 949-67-7**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(esterification of, with [(chlorobenzoyl)phenoxy]methylpropanoyl chloride)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 949-67-7 HCAPLUS
CN L-Tyrosine, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



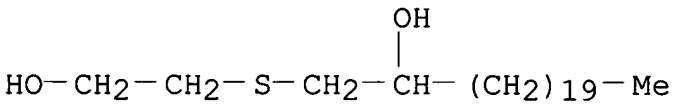
IC C07C; A61K
CC 25-19 (Noncondensed Aromatic Compounds)
IT 105-59-9 **111-48-8** 623-50-7 **949-67-7**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(esterification of, with [(chlorobenzoyl)phenoxy]methylpropanoyl chloride)

L48 ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1979:187977 Document No. 90:187977 Phenol group-containing sugar **alcohol** phosphites and phosphates. Mayer, Norbert; Pfahler, Gerhard; Wiezer, Hartmut (Hoechst A.-G., Fed. Rep. Ger.). Ger. Offen. DE 2738675 19790308, 39 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1977-2738675 19770827.
AB Mixed esters, useful as stabilizers for polymers such as PVC [9002-86-2] and polypropylene [9003-07-0], are prepared by the reaction of phosphite ester, such as P(OEt)3, with a polyhydric **alc.** such as sorbitol or xylitol, a phenol group-containing compound such as 3,3-bis(3-tert-butyl-4-hydroxyphenyl)-1-butanol (I), or 4-[(dimethylamino)methyl]-2,6-di-tert-butylphenol, 2,5-di-tert-butylhydroquinone, or 2,2-bis(3-tert-butyl-4-hydroxyphenyl)butanoic acid hydrazide, and compound such as 1,2-triacontanediol (II), stearyl **alc.** (III), 3-thiapentaeicosane-1,5-diol, glycerol monostearate, and/or

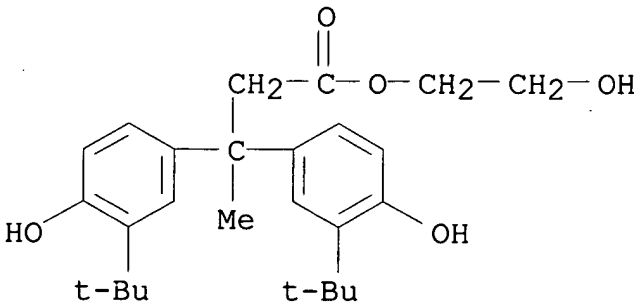
stearylamine. The mixed esters have good resistance to hydrolysis. Thus, a mixture of I 0.1, II 0.1, III 0.1, sorbitol 0.1, and P(OEt)3 0.315 mol containing Et3N catalyst is heated with distillation of EtOH to give 105 g mixed ester.

IT **70140-62-4D**, esters with phenols and phosphorous acid
70140-64-6D, esters with phosphorous acid and polyols
70140-65-7D, esters with phosphorous acid and polyols
70215-34-8D, esters with phenols and phosphorous acid
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(stabilizers, for polymers)

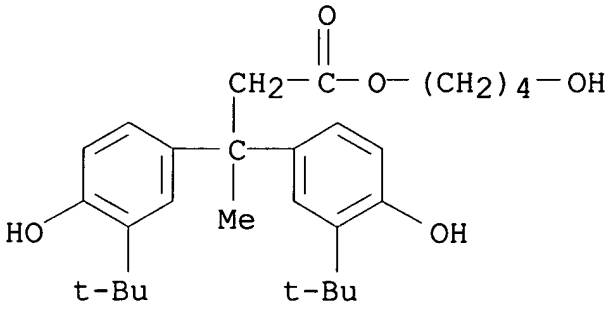
RN 70140-62-4 HCAPLUS
CN 2-Docosanol, 1-[(2-hydroxyethyl)thio]- (9CI) (CA INDEX NAME)



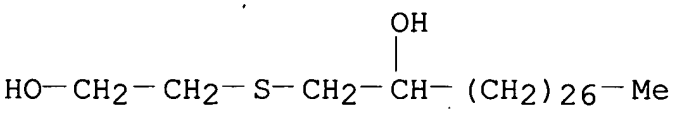
RN 70140-64-6 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-β-[3-(1,1-dimethylethyl)-4-hydroxyphenyl]-4-hydroxy-β-methyl-, 2-hydroxyethyl ester (9CI) (CA INDEX NAME)



RN 70140-65-7 HCAPLUS
CN Benzenepropanoic acid, 3-(1,1-dimethylethyl)-β-[3-(1,1-dimethylethyl)-4-hydroxyphenyl]-4-hydroxy-β-methyl-, 4-hydroxybutyl ester (9CI) (CA INDEX NAME)

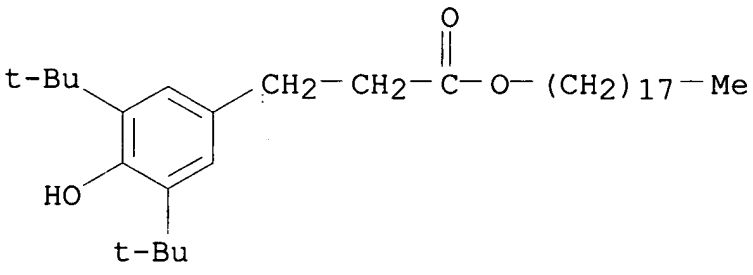


RN 70215-34-8 HCAPLUS
CN 2-Nonacosanol, 1-[(2-hydroxyethyl)thio]- (9CI) (CA INDEX NAME)



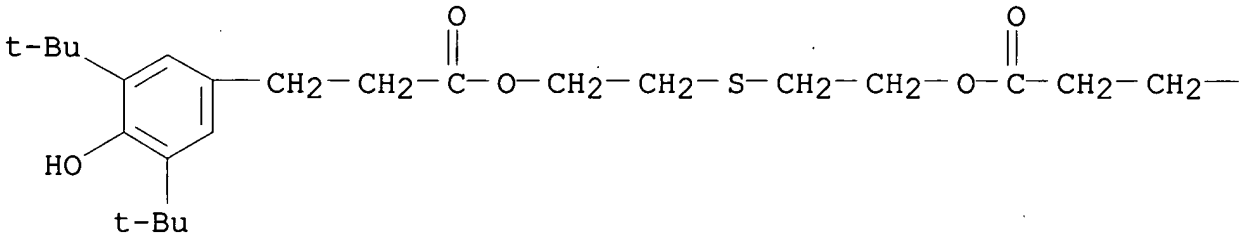
IC C07F009-15
CC 36-6 (Plastics Manufacture and Processing)
IT 50-70-4D, esters with phenols and phosphorous acid 69-65-8D, esters with phenols and phosphorous acid 87-99-0D, esters with phenols and phosphorous acid 88-27-7D, esters with phosphorous acid and polyols 88-58-4D, esters with phosphorous acid and polyols 98-29-3D, esters with phosphorous acid and polyols 101-02-0D, reaction products with polyols and phenolic compds. 121-45-9D, reaction products with polyols and phenolic compds. 122-52-1D, reaction products with polyols and phenolic compds. 124-30-1D, reaction products with phosphite esters of phenols and polyols 149-32-6D, esters with phenols and phosphorous acid 608-66-2D, esters with phenols and phosphorous acid 868-85-9D, reaction products with polyols and phenolic compds. 1020-31-1D, esters with phosphorous acid and polyols 31566-31-1D, esters with phenols and phosphorous acid 36294-23-2D, esters with phosphorous acid and polyols 66063-40-9D, esters with phenols and phosphorous acid 68461-53-0D, reaction products with polyol phosphites **70140-62-4D**, esters with phenols and phosphorous acid 70140-63-5D, esters with phosphorous acid and polyols **70140-64-6D**, esters with phosphorous acid and polyols **70140-65-7D**, esters with phosphorous acid and polyols **70215-34-8D**, esters with phenols and phosphorous acid
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(stabilizers, for polymers)

L48 ANSWER 22 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1974:520262 Document No. 81:120262 3-(3,5-Di-tert-butyl-4-hydroxyphenyl)propionates. Park, Kyong P.; Vellturo, Anthony F. (Ciba-Geigy A.-G.). Ger. Offen. DE 2364121 19740711, 18 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1973-2364121 19731221.
GI For diagram(s), see printed CA Issue.
AB RC18H37-n (I) and (RCH2CH2)2S, useful as antioxidants for organic materials, were prepared by reaction of CH2:CHCO2Me (II) with 2,6-(Me3C)2C6H3OH (III) and the corresponding **alcs.** in the presence of MeONa or Me3COK. Thus, II was added to a mixture of III, n-C18H37OH, and MeONa at 105-8° and heated at 130° to give 80% I.
IT **2082-79-3P 41484-35-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2082-79-3 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (9CI) (CA INDEX NAME)

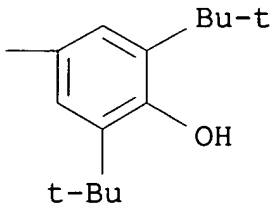


RN 41484-35-9 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

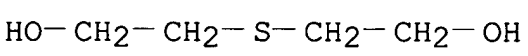
PAGE 1-A



PAGE 1-B



IT **111-48-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with di-tert-butylphenol and methyl acrylate)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



IC C07C; C08F
CC 25-18 (Noncondensed Aromatic Compounds)
IT Catalysts and Catalysis
(alkali metal alkoxides, for methyl acrylate reaction with di-tert-butylphenol and **alcs**.)
IT 124-41-4 865-47-4
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for methyl acrylate reaction with di-tert-butylphenol and **alcs**.)
IT **2082-79-3P 41484-35-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 96-33-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with di-tert-butylphenol and **alcs**.)
IT **111-48-8** 112-92-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with di-tert-butylphenol and methyl acrylate)
IT 128-39-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyl acrylate and octadecyl **alc**. (or thiodiglycol))

L48 ANSWER 23 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1974:520260 Document No. 81:120260 3-(3,5-Di-tert-butyl-4-hydroxyphenyl)propionates. Haeberli, Joerg; Park, Kyong P.; Vellturo, Anthony F.; Nurnberger, George F. (Ciba-Geigy A.-G.).

Ger. Offen. DE 2364126 19740711, 28 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1973-2364126 19731221.

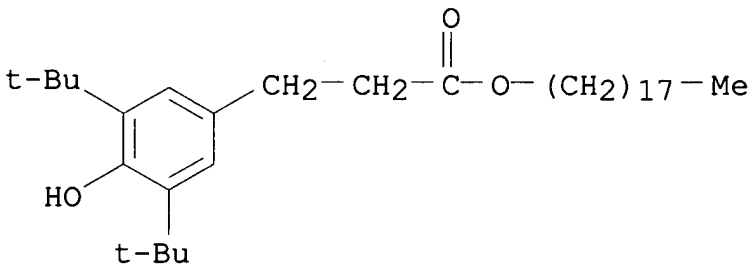
GI For diagram(s), see printed CA Issue.

AB (RCH2CH2)2S (I), RC18H37-n, and (RCH2)4C, useful asantioxidants for organic materials, were prepared by reaction of 2,6-(Me3C)2C6H3OH (II) with CH2:CHCO2Me (III) in thepresence of Me3COK or MeONa, followed by reaction with **alcs.** in the presence of LiOH or LiNH2. Thus, II was treated with III in Me2CHOH in the presence of Me3COK at 110°, and after removal of excess III, the product was treated with (HOCH2CH2)2S in the presence of LiOH.H2O at ≤145° to give 75.4% I.

IT **2082-79-3P 41484-35-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 2082-79-3 HCAPLUS

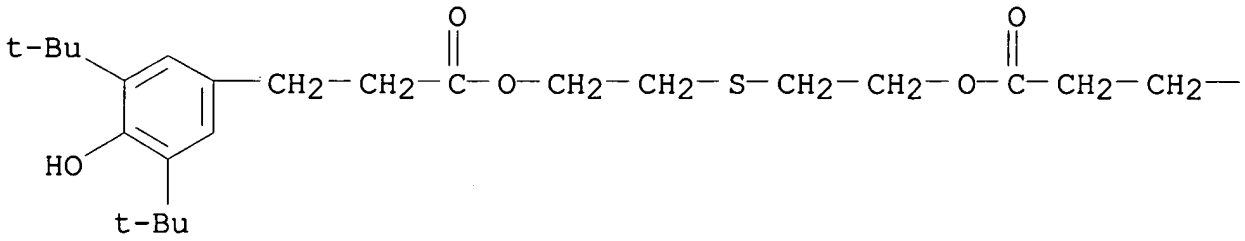
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (9CI) (CA INDEX NAME)



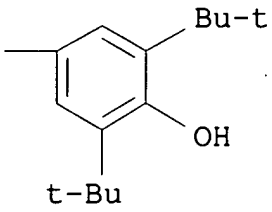
RN 41484-35-9 HCAPLUS

CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT **111-48-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with reaction product of di-tert-butylphenol and methyl acrylate)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

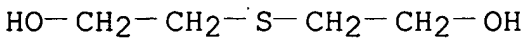
HO—CH_2—CH_2—S—CH_2—CH_2—OH

IC C07C; C08F
CC 25-18 (Noncondensed Aromatic Compounds)
IT Transesterification catalysts
(lithium compds., for methyl (di-tert-butylhydroxyphenyl)propionate with **alcs**.)
IT 1310-65-2 7782-89-0
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for transesterification of methyl (di-tert-butylhydroxyphenyl)propionate with **alcs**.)
IT **2082-79-3P 41484-35-9P** 53423-24-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **111-48-8** 112-92-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with reaction product of di-tert-butylphenol and methyl acrylate)

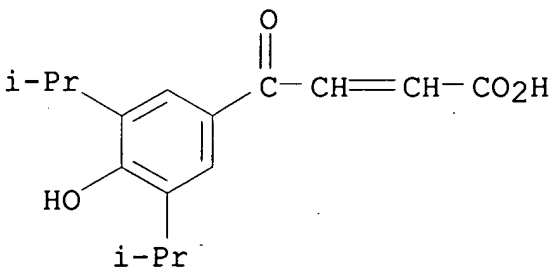
L48 ANSWER 24 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1974:403608 Document No. 81:3608 Hydroxybenzoyl carboxylic acid ester. Schmidt, Andreas (Ciba-Geigy A.-G.). Ger. Offen. DE 2341125 19740228, 73 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1973-2341125 19730814.
GI For diagram(s), see printed CA Issue.
AB Esters I, II, III, and IV (R = Me, Me2CH, EtCHMe; Z = CH2CH2, CH:CH; R1 = e.g., Me, Et, Bu, C18H37; R2 = e.g., C8H17, C12H25) were useful as stabilizers for polymers, e.g., polypropylene.

Thus, 2,6-Me2C6H3OH reacted with maleic anhydride and AlCl3 to give 3,5,4-Me2(HO)C6H2COCH:CHCO2H (V) which was reduced to 3,5,4-Me2(HO)C6H2COCH2-CH2CO2H (VI). V reacted with C8H17SH in MeOH-Et3N to give 3,5,4-Me2(HO)C6H2COCH2CH(SC8H17)CO2H (VII). V, VI, and VII were esterified with **alcs.** to give the corresponding esters. The octadecyl ester of VI reacted with HSCH2CH2SH to give IV (R = Me, R1 = C18H37). About 40 compds. were prepared

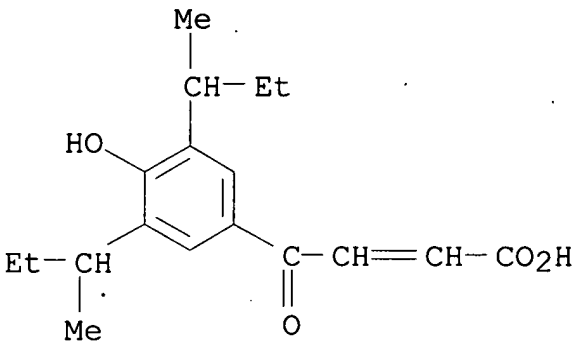
IT **111-48-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification by, of benzoylacrylic and propionic acids)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



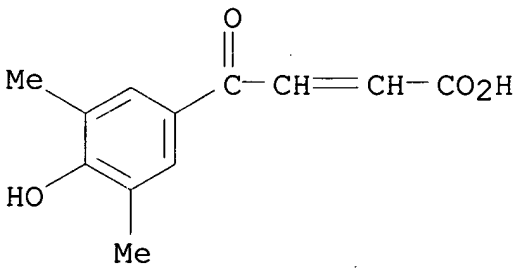
IT **52245-96-2P 52245-97-3P 52245-98-4P**
52245-99-5P 52246-00-1P 52246-01-2P
52246-03-4P 52246-04-5P 52246-05-6P
52246-06-7P 52246-07-8P 52246-08-9P
52246-09-0P 52246-10-3P 52246-11-4P
52246-12-5P 52246-14-7P 52246-15-8P
52246-16-9P 52246-17-0P 52246-18-1P
52246-19-2P 52246-20-5P 52246-21-6P
52246-22-7P 52246-23-8P 52246-24-9P
52246-25-0P 52246-26-1P 52246-27-2P
52246-30-7P 52246-31-8P 52246-32-9P
52365-71-6P 52365-72-7P 52365-73-8P
52365-74-9P 52478-54-3P 52810-87-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52245-96-2 HCAPLUS
CN 2-Butenoic acid, 4-[4-hydroxy-3,5-bis(1-methylethyl)phenyl]-4-oxo- (9CI) (CA INDEX NAME)



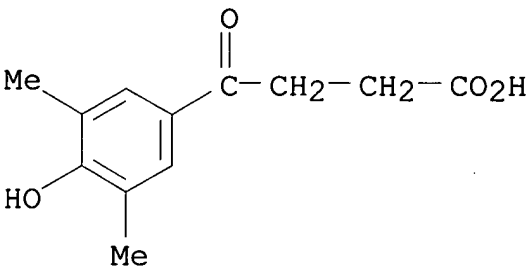
RN 52245-97-3 HCAPLUS
CN 2-Butenoic acid, 4-[4-hydroxy-3,5-bis(1-methylpropyl)phenyl]-4-oxo- (9CI) (CA INDEX NAME)



RN 52245-98-4 HCAPLUS
CN 2-Butenoic acid, 4-(4-hydroxy-3,5-dimethylphenyl)-4-oxo- (9CI) (CA INDEX NAME)

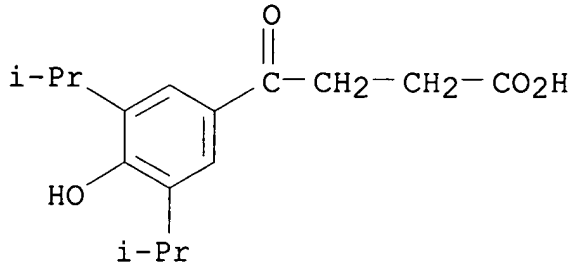


RN 52245-99-5 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-γ-oxo- (9CI) (CA INDEX NAME)

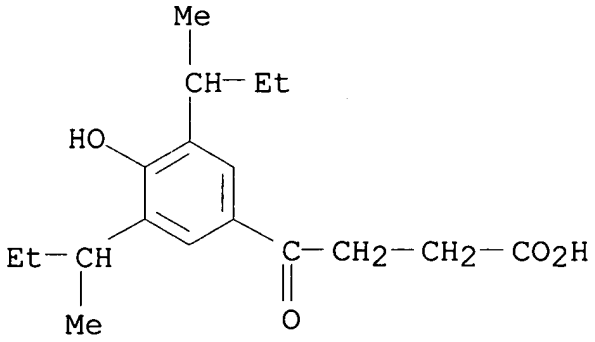


RN 52246-00-1 HCAPLUS

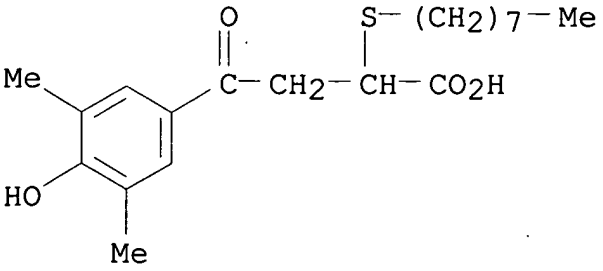
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo- (9CI) (CA INDEX NAME)



RN 52246-01-2 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylpropyl)-γ-oxo- (9CI) (CA INDEX NAME)

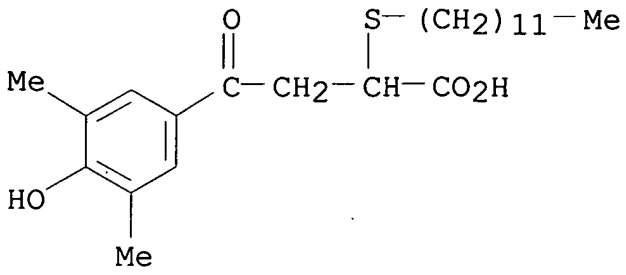


RN 52246-03-4 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-α-(octylthio)-γ-oxo- (9CI) (CA INDEX NAME)

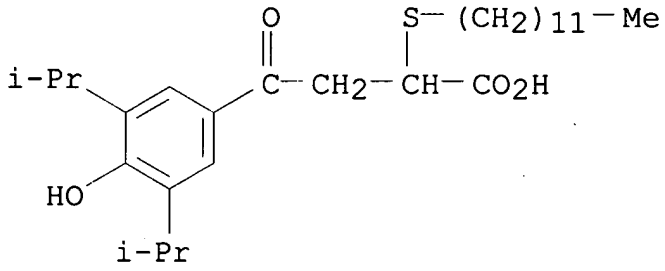


RN 52246-04-5 HCAPLUS
CN Benzenebutanoic acid, α-(dodecylthio)-4-hydroxy-3,5-dimethyl-

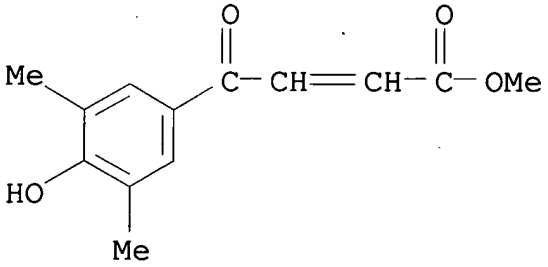
γ-oxo- (9CI) (CA INDEX NAME)



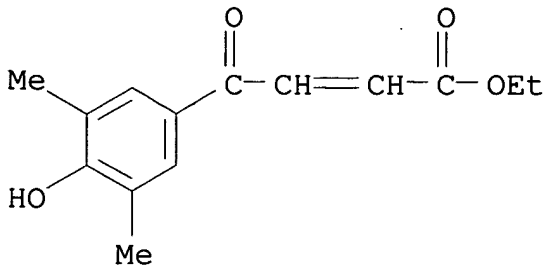
RN 52246-05-6 HCAPLUS
CN Benzenebutanoic acid, α-(dodecylthio)-4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo- (9CI) (CA INDEX NAME)



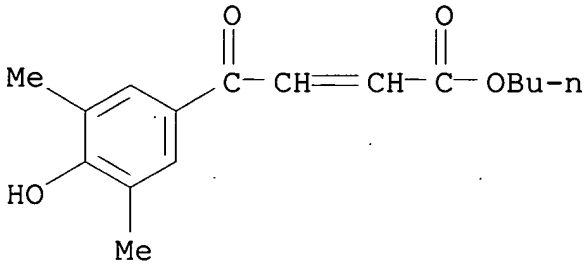
RN 52246-06-7 HCAPLUS
CN 2-Butenoic acid, 4-(4-hydroxy-3,5-dimethylphenyl)-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



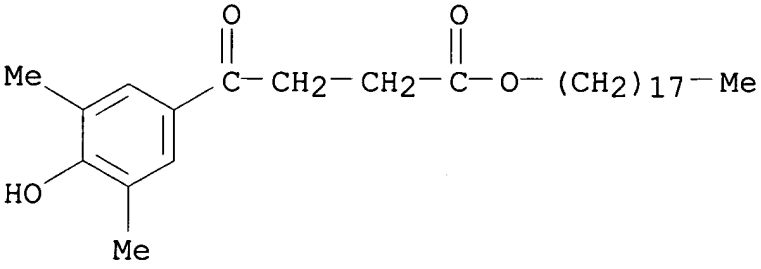
RN 52246-07-8 HCAPLUS
CN 2-Butenoic acid, 4-(4-hydroxy-3,5-dimethylphenyl)-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



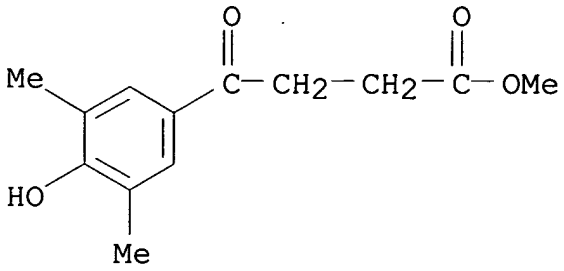
RN 52246-08-9 HCAPLUS
CN 2-Butenoic acid, 4-(4-hydroxy-3,5-dimethylphenyl)-4-oxo-, butyl ester (9CI) (CA INDEX NAME)



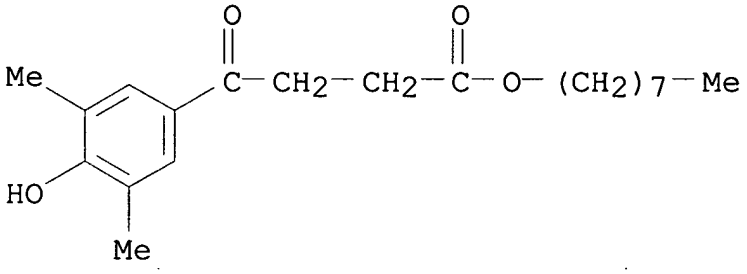
RN 52246-09-0 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-γ-oxo-, octadecyl ester (9CI) (CA INDEX NAME)



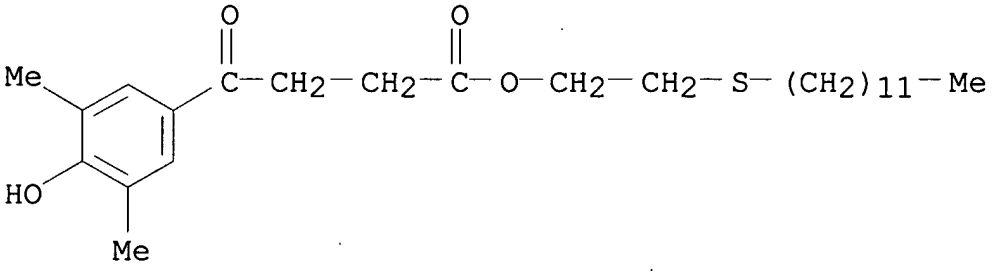
RN 52246-10-3 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-γ-oxo-, methyl ester (9CI) (CA INDEX NAME)



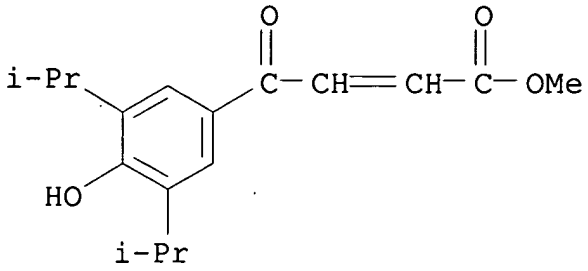
RN 52246-11-4 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-γ-oxo-, octyl ester (9CI) (CA INDEX NAME)



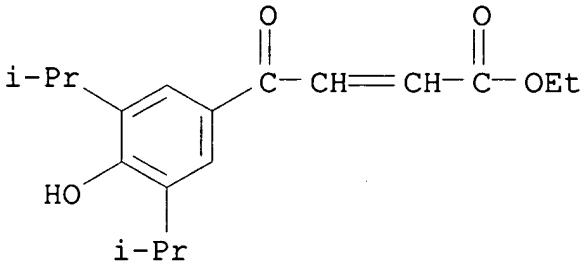
RN 52246-12-5 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-γ-oxo-, 2-(dodecylthio)ethyl ester (9CI) (CA INDEX NAME)



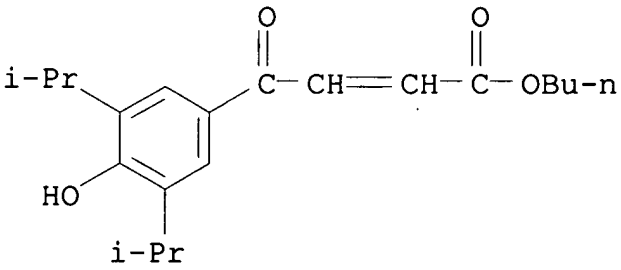
RN 52246-14-7 HCAPLUS
CN 2-Butenoic acid, 4-[4-hydroxy-3,5-bis(1-methylethyl)phenyl]-4-oxo-, methyl ester (9CI) (CA INDEX NAME)



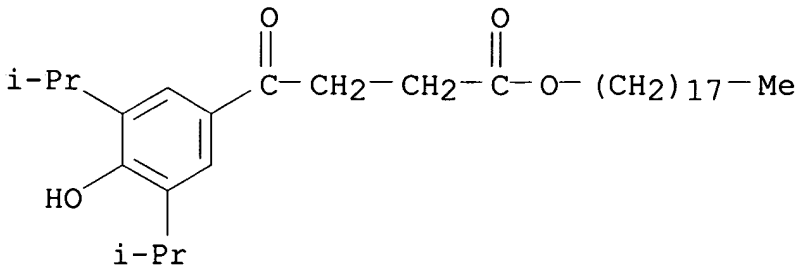
RN 52246-15-8 HCAPLUS
CN 2-Butenoic acid, 4-[4-hydroxy-3,5-bis(1-methylethyl)phenyl]-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



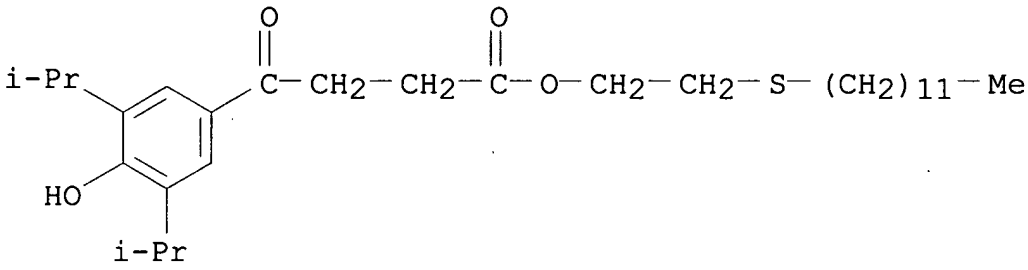
RN 52246-16-9 HCAPLUS
CN 2-Butenoic acid, 4-[4-hydroxy-3,5-bis(1-methylethyl)phenyl]-4-oxo-, butyl ester (9CI) (CA INDEX NAME)



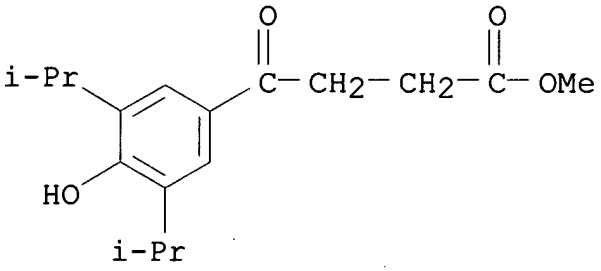
RN 52246-17-0 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo-, octadecyl ester (9CI) (CA INDEX NAME)



RN 52246-18-1 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo-, 2-(dodecylthio)ethyl ester (9CI) (CA INDEX NAME)



RN 52246-19-2 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 52246-20-5 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)

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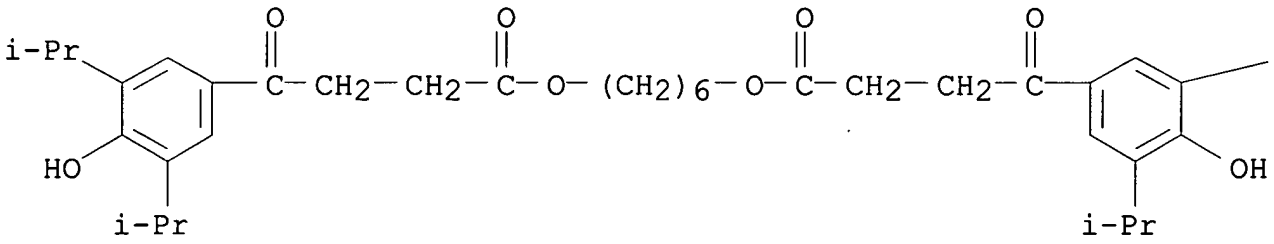

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RN 52246-21-6 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

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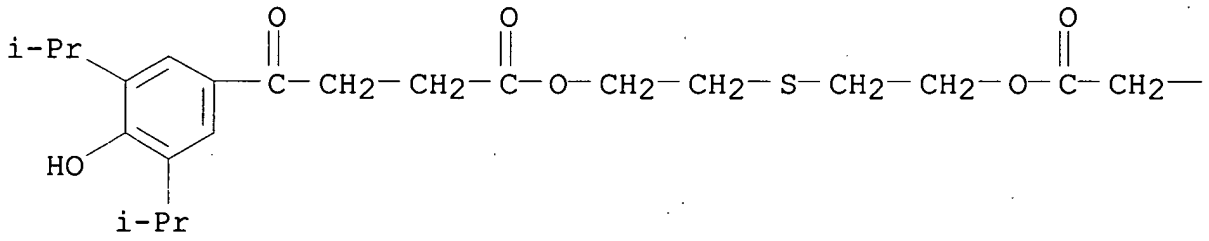

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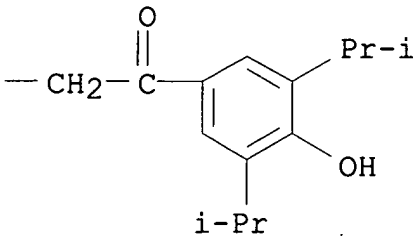
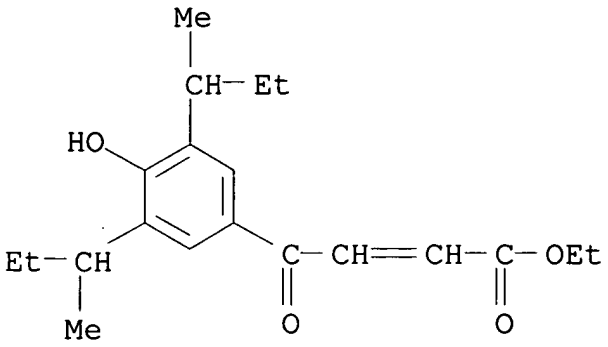
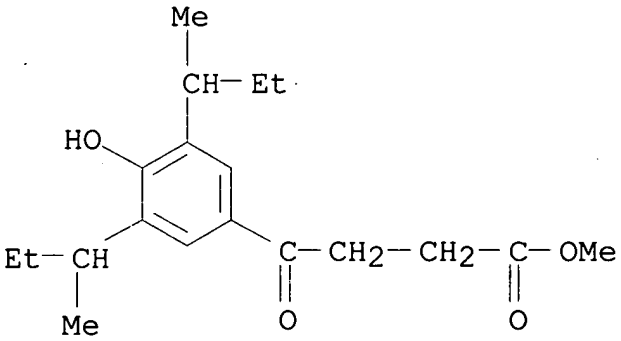


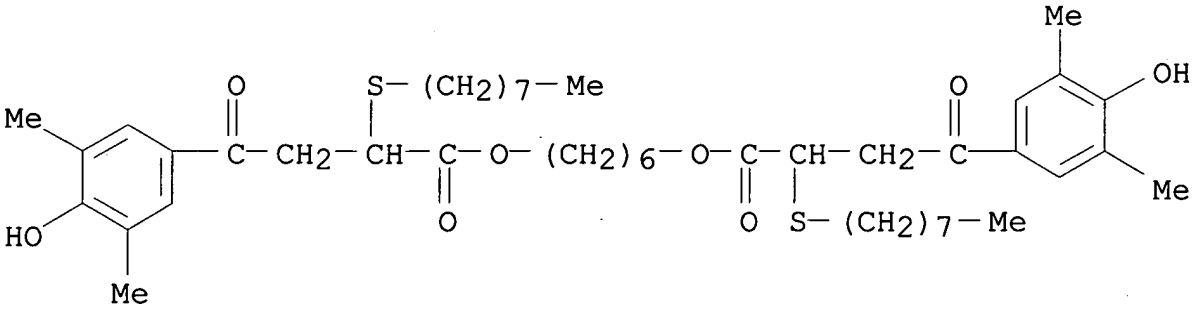
RN 52246-22-7 HCAPLUS
CN 2-Butenoic acid, 4-[4-hydroxy-3,5-bis(1-methylpropyl)phenyl]-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)



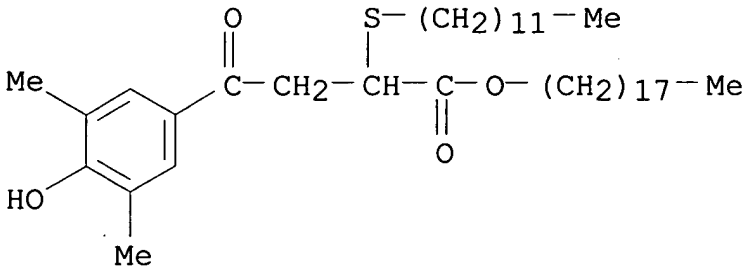
RN 52246-23-8 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylpropyl)-γ-oxo-, methyl ester (9CI) (CA INDEX NAME)



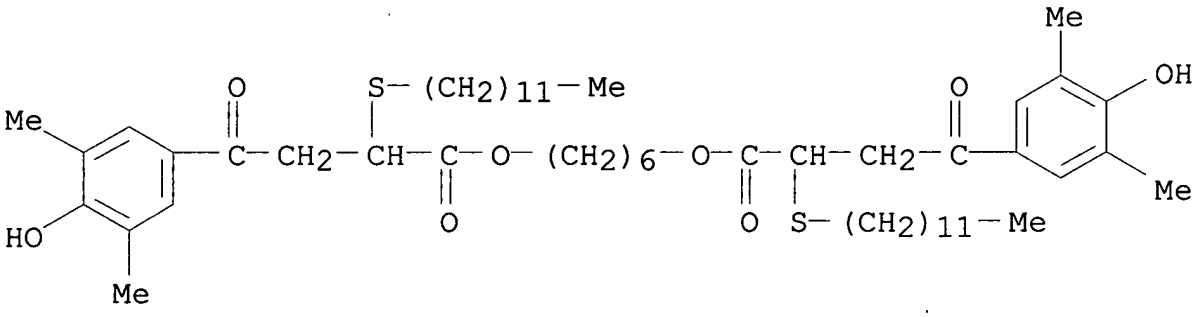
RN 52246-24-9 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-α-(octylthio)-γ-oxo-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)



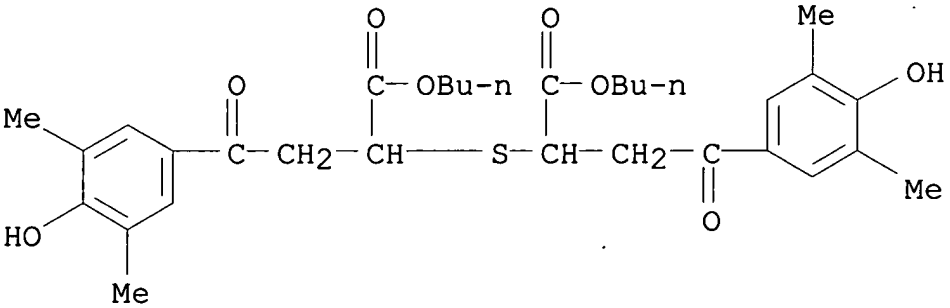
RN 52246-25-0 HCAPLUS
CN Benzenebutanoic acid, α-(dodecylthio)-4-hydroxy-3,5-dimethyl-γ-oxo-, octadecyl ester (9CI) (CA INDEX NAME)



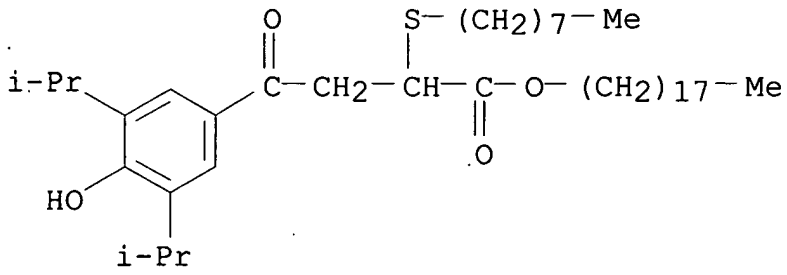
RN 52246-26-1 HCAPLUS
CN Benzenebutanoic acid, α-(dodecylthio)-4-hydroxy-3,5-dimethyl-γ-oxo-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)



RN 52246-27-2 HCAPLUS
CN Benzenebutanoic acid, α,α'-thiobis[4-hydroxy-3,5-dimethyl-γ-oxo-, dibutyl ester (9CI) (CA INDEX NAME)



RN 52246-30-7 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-α-(octylthio)-γ-oxo-, octadecyl ester (9CI) (CA INDEX NAME)



RN 52246-31-8 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-α-(octylthio)-γ-oxo-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)

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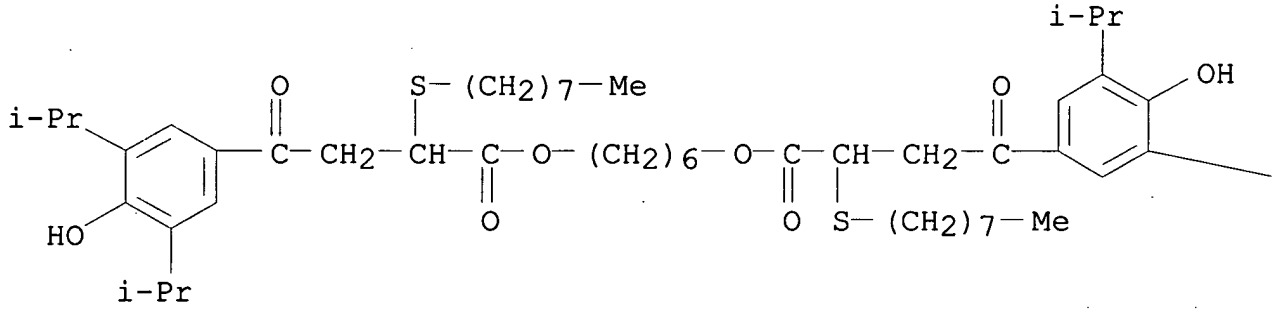

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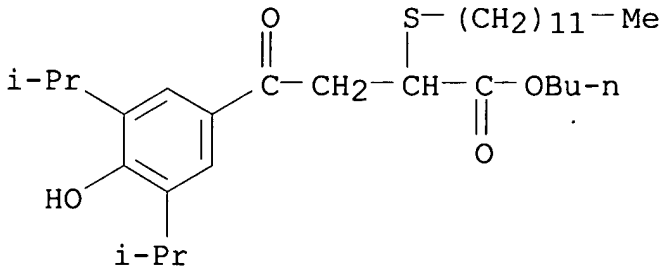
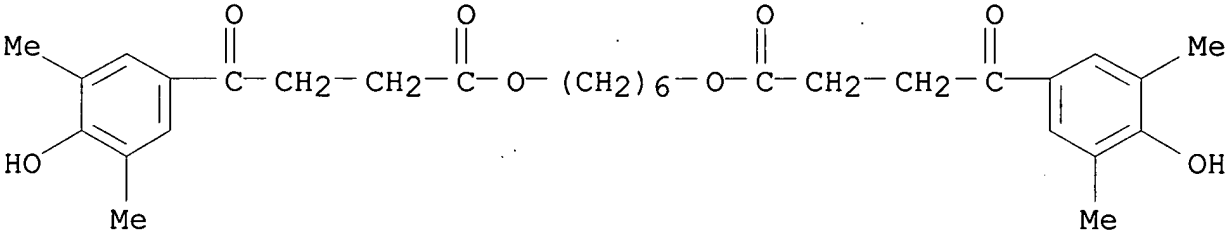
RN 52246-32-9 HCAPLUS
CN Benzenebutanoic acid, α-(dodecylthio)-4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo-, butyl ester (9CI) (CA INDEX NAME)



RN 52365-71-6 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-γ-oxo-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)



RN 52365-72-7 HCAPLUS
CN Benzenebutanoic acid, 4-hydroxy-3,5-dimethyl-γ-oxo-, 2,2-bis[[4-(4-hydroxy-3,5-dimethylphenyl)-1,4-dioxobutoxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

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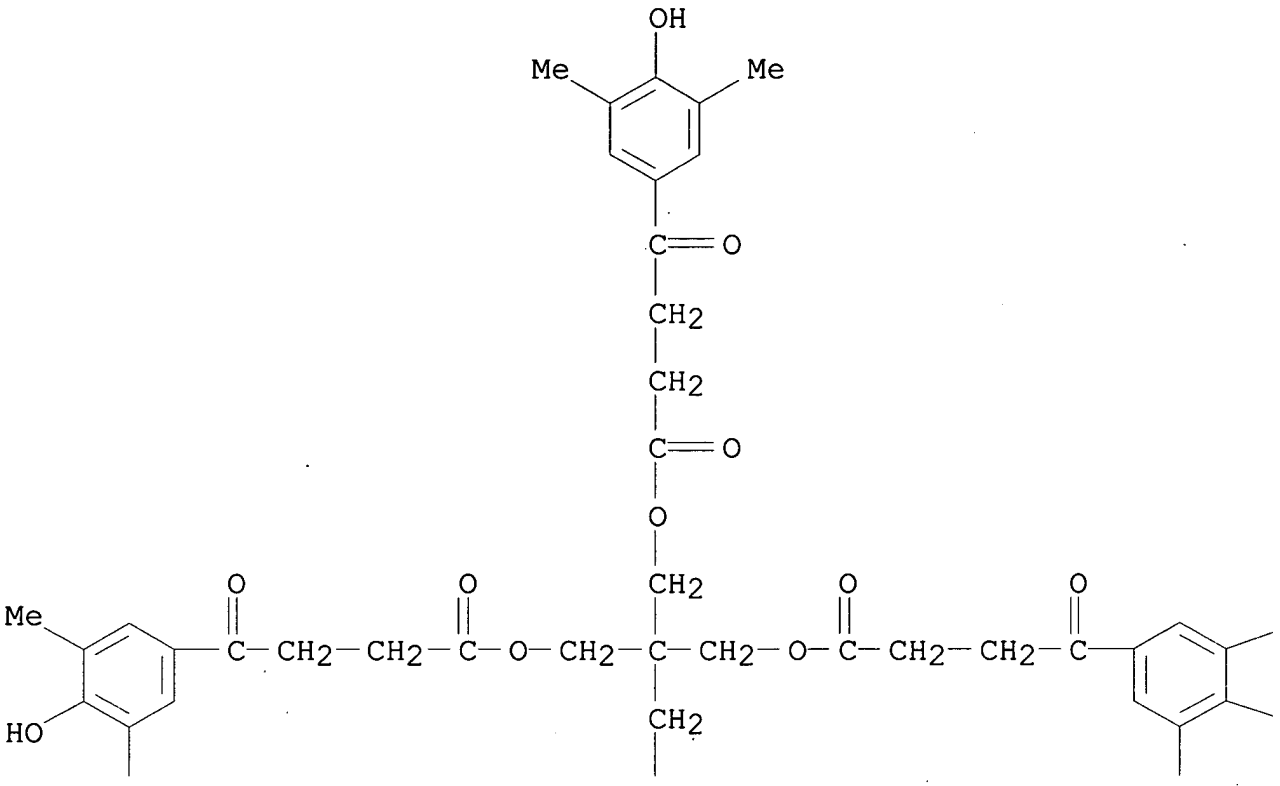
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C
O
CH2
CH2
C
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O
CH2
CH2
Me
HO
O
C
CH2
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CH2
CH2
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O
C
CH2
CH2
C
O

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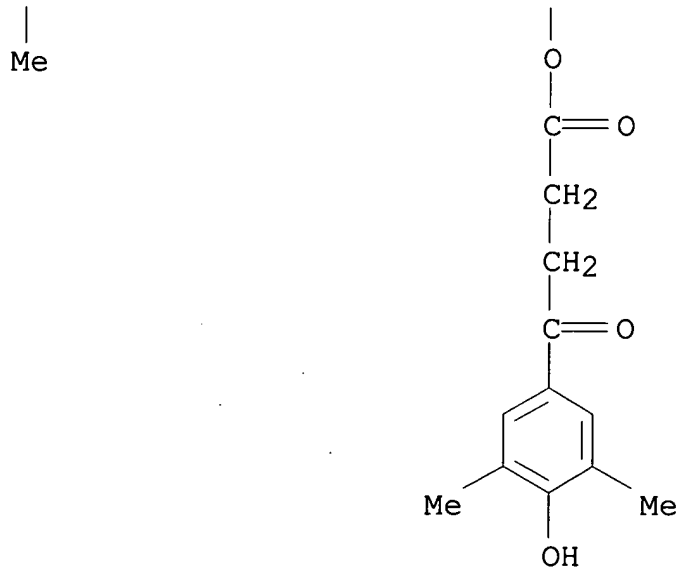
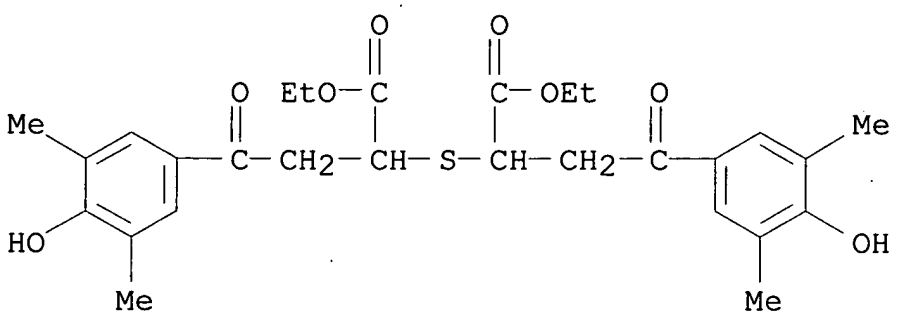
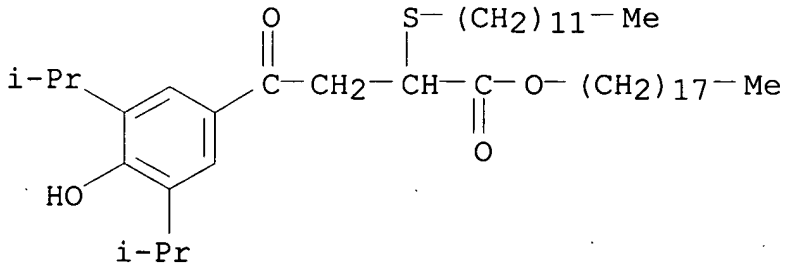


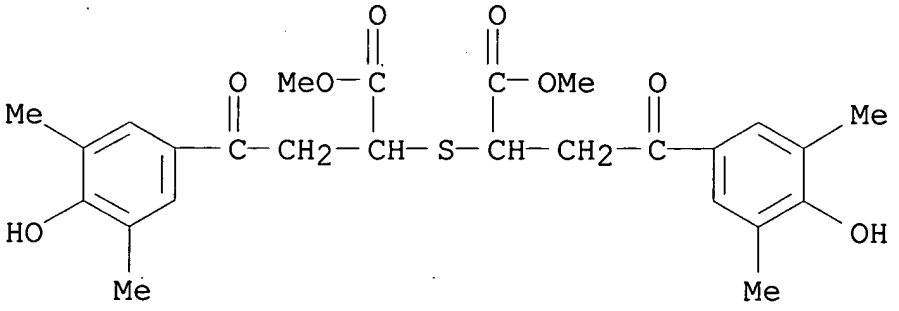
RN 52365-73-8 HCAPLUS
CN Benzenebutanoic acid, α,α'-thiobis[4-hydroxy-3,5-dimethyl-γ-oxo-, diethyl ester (9CI) (CA INDEX NAME)



RN 52365-74-9 HCAPLUS
CN Benzenebutanoic acid, α-(dodecylthio)-4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo-, octadecyl ester (9CI) (CA INDEX NAME)



RN 52478-54-3 HCAPLUS
CN Benzenebutanoic acid, α,α'-thiobis[4-hydroxy-3,5-dimethyl-γ-oxo-, dimethyl ester (9CI) (CA INDEX NAME)



RN 52810-87-4 HCAPLUS

CN Benzenebutanoic acid, 4-hydroxy-3,5-bis(1-methylethyl)-γ-oxo-, 2,2-bis[[4-[4-hydroxy-3,5-bis(1-methylethyl)phenyl]-1,4-dioxobutoxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

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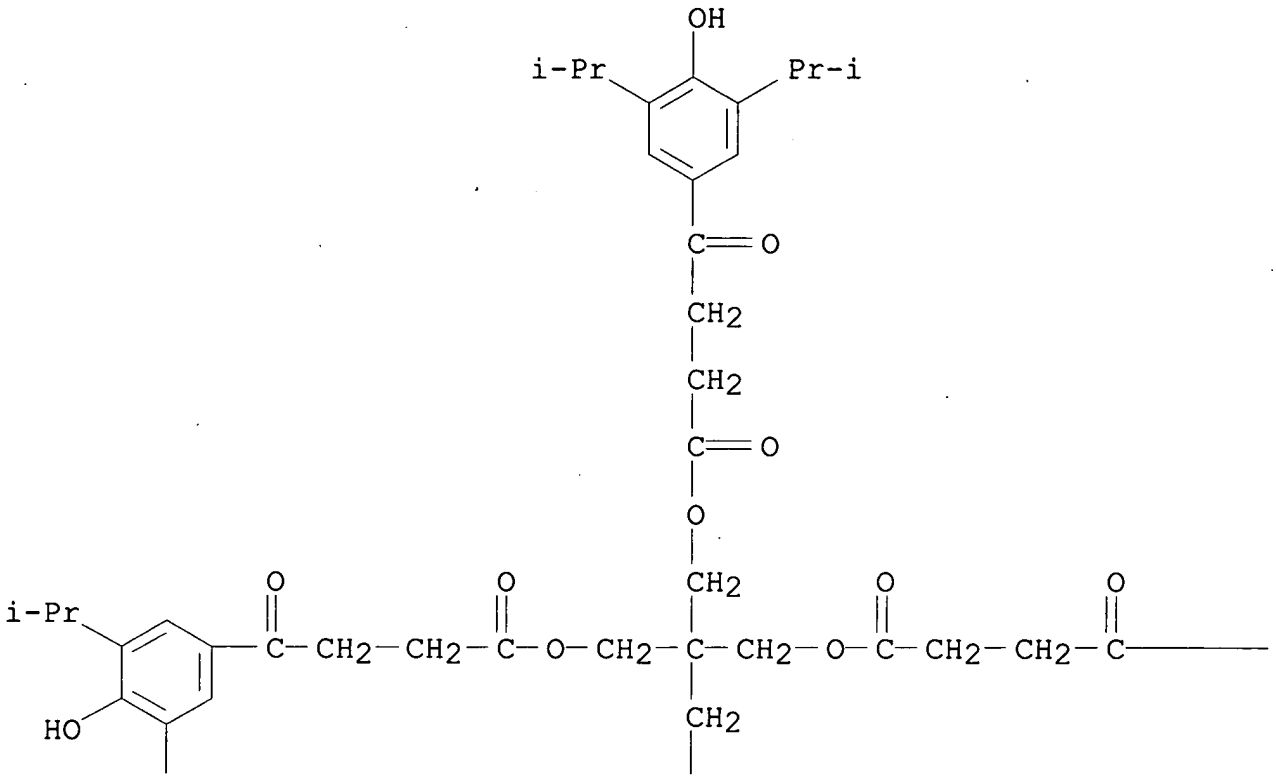

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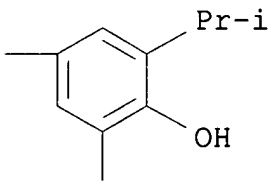
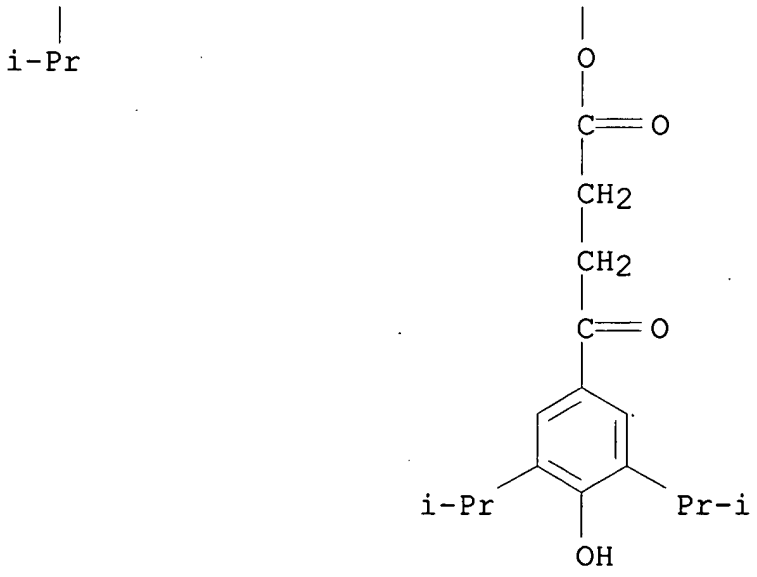


PAGE 2-A



PAGE 2-B

i-Pr

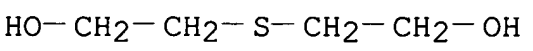
IC C07C; C07D; B01J; C08F
CC 25-18 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 35
IT 64-17-5, reactions 67-56-1, reactions 71-36-3, reactions
111-48-8 112-92-5 126-30-7 629-11-8 1462-55-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification by, of benzoylacrylic and propionic acids)
IT **52245-96-2P 52245-97-3P 52245-98-4P**
52245-99-5P 52246-00-1P 52246-01-2P
52246-02-3P **52246-03-4P 52246-04-5P**
52246-05-6P 52246-06-7P 52246-07-8P
52246-08-9P 52246-09-0P 52246-10-3P
52246-11-4P 52246-12-5P 52246-13-6P
52246-14-7P 52246-15-8P 52246-16-9P
52246-17-0P 52246-18-1P 52246-19-2P
52246-20-5P 52246-21-6P 52246-22-7P
52246-23-8P 52246-24-9P 52246-25-0P
52246-26-1P 52246-27-2P 52246-28-3P
52246-29-4P **52246-30-7P 52246-31-8P**
52246-32-9P 52246-33-0P **52365-71-6P**
52365-72-7P 52365-73-8P 52365-74-9P
52365-75-0P **52478-54-3P 52810-87-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L48 ANSWER 25 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1970:478120 Document No. 73:78120 Organotin compounds as stabilizers for polymeric compositions. (Imperial Chemical Industries Ltd.). Fr. FR 1581953 19690919, 24 pp. (French). CODEN: FRXXAK.
APPLICATION: FR 1968-167979 19680927.
AB An alkyltin oxide is treated with an organic composition containing an active
H to give a stabilizer used to prevent thermal degradation in polymers. Thus, trimethylolpropane trimaleate 4.28, ethylene glycol bis(2-mercaptopropionate) 7.15, cyclohexyl maleate (I) 5.58, and Bu2SnO 14.9 parts, were refluxed in 200 ml PhMe to give 28 parts of a pale brown viscous oil. The oil (1 part) was mixed with 100 parts poly(vinyl chloride) containing 0.25 part stearic acid and the polymer was stable and colorless after ≤40 min at 175°. In the absence of a stabilizer the same polymer

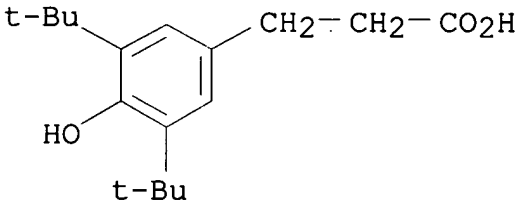
turned black after 20 min. Similar compns. were prepared using lauric acid, lauryl **alc.**, or lauryl mercaptan in place of I, and dioctyltin oxide.

IT **111-48-8 20170-32-5**
RL: USES (Uses)
(reaction products with stannanes, stabilizers, for chloroethylene polymers)

RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 20170-32-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy- (9CI) (CA INDEX NAME)



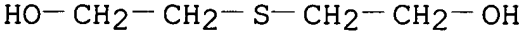
IC C08F
CC 36 (Plastics Manufacture and Processing)
IT 79-42-5 98-91-9 111-29-5 **111-48-8** 112-53-8 112-55-0 126-30-7 1892-29-1 2424-59-1 3570-55-6 3746-39-2 7659-86-1 14440-77-8 15498-42-7 **20170-32-5** 27309-95-1 28574-65-4 29275-72-7 29275-73-8 29275-74-9 29275-75-0 29275-76-1 29275-77-2 29275-79-4 29303-14-8 29367-13-3
RL: USES (Uses)
(reaction products with stannanes, stabilizers, for chloroethylene polymers)

L48 ANSWER 26 OF 26 HCAPLUS COPYRIGHT 2005 ACS on STN
1964:16442 Document No. 60:16442 Original Reference No. 60:2854e-g Stabilization of organic materials. Dexter, Martin; Spivack, John D.; Steinberg, David H. (J. R. Geigy A.-G.). FR 1337163 19630906, 29 pp. (Unavailable). PRIORITY: US 19611030.

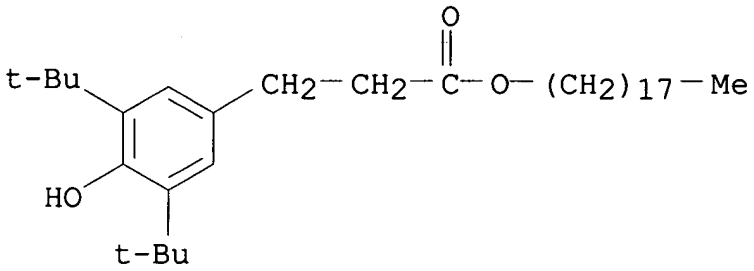
AB Esters prepared from carboxylic acids substituted by the 3,5-di-tert-butyl-4-hydroxyphenyl group were effective stabilizers for organic materials, e.g. polymers and mineral oil, against oxidative degradation. The esters were prepared by the following

standard methods: A. Base catalyzed ester exchange of the Me ester. B. Acid catalyzed esterification. C. Reaction of a β-chloroalkyl sulfide with the Na salt of a carboxylic acid. D. Reaction of a carboxylic acid chloride with an **alc**. The following [3,5,4-(tert-Bu)2(HO)C6H2]nZ were prepared (method, n, Z, b.p./mm., and m.p. given): A, 1, CH2CO2C18H37-n, 230°/0.075, 33-5°; A, 1, CO2C18H37-n, --, 65-7°; A, 1, CO2CH2CH2SCH2CH2OH, --, 114-15°; A, 2, (CH2CO2CH2CH2)2S, --, 117-18°; B, 1, CH2CH2CO2C18H37-n , --, 49-50°; B, 2, (CH2CH2CO2CH2CH2)2O, --, 90-1.5°; B, 2, CH2CH2CO2CHMeCH2O2CCH2CH2, --, 70°; B, 2, (CH2CH2CO2)2(CH2)2, --, 146-7°; C, 1, CO2CH2CH2SC8H17, 206-8°/0.14, -- (n26.5D 1.5128); C, 1, CH2CO2CH2CH2SC8H17 207°/0.07, -- (n27.2D 1.5085); C, 1, CH2CO2CH2CH2SC18H37, --, -- ; C, 1, CO2CH2CH2SC18H37,--, --; D, 1, CO2C6H13-n, 150-5°/0.1, 70-2°; D, 1, CO2C12H25-n, 189-93°/1-2, 47-53°. As an example of the stabilizing effect of the esters, a polypropylene film containing 0.5% by weight of 2-(n-octadecylthioethyl) 3,5-di-tert-butyl-4-hydroxyphenylacetate was unchanged after 1000 hrs. at 149° in a forced-air oven. The unstabilized polymer was altered after only 3 hrs.

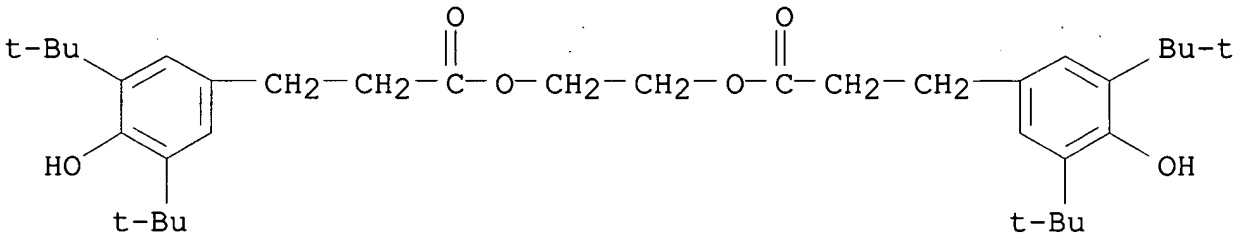
IT **111-48-8**, Ethanol, 2,2'-thiodi-
(esters)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



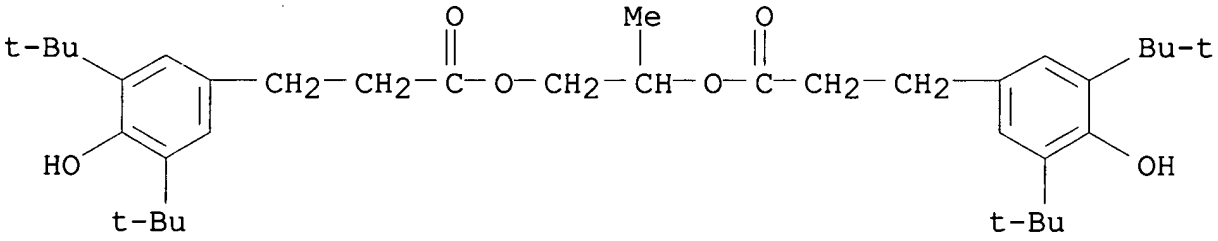
IT **2082-79-3**, Hydrocinnamic acid, 3,5-di-tert-butyl-4-hydroxy-, octadecyl ester **6524-49-8**, Ethylene glycol, bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate) **35455-13-1**, 1,2-Propanediol, bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate) **38879-22-0**, Diethylene glycol, 3,5-di-tert-butyl-4-hydroxyhydrocinnamate
(preparation of)
RN 2082-79-3 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (9CI) (CA INDEX NAME)



RN 6524-49-8 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1,2-ethanediyl ester (9CI) (CA INDEX NAME)

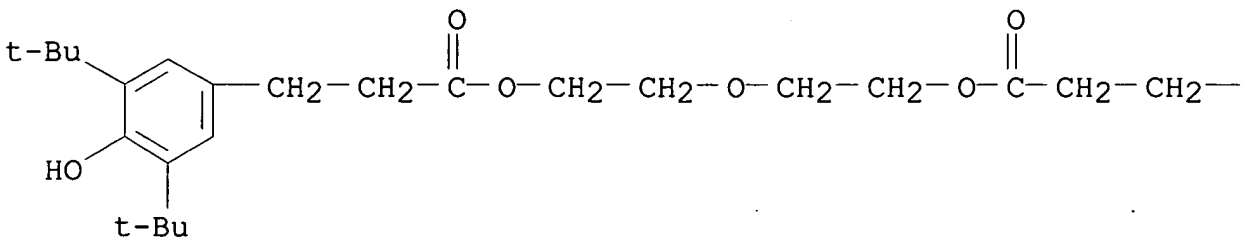


RN 35455-13-1 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 1-methyl-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

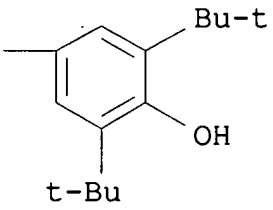


RN 38879-22-0 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, oxydi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IC C07C; C08F
CC 35 (Noncondensed Aromatic Compounds)
IT **111-48-8**, Ethanol, 2,2'-thiodi- 3547-33-9, Ethanol, 2-(octylthio)- 26535-62-6, Ethanol, 2-(octadecylthio)- (esters)
IT **2082-79-3**, Hydrocinnamic acid, 3,5-di-tert-butyl-4-hydroxy-, octadecyl ester 4221-75-4, Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-, dodecyl ester 6386-41-0, Acetic acid, (3,5-di-tert-butyl-4-hydroxyphenyl)-, methyl ester **6524-49-8**, Ethylene glycol, bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate) 7664-53-1, Acetic acid, (3,5-di-tert-butyl-4-hydroxyphenyl)-, octadecyl ester 7664-56-4, Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-, 2-(octadecylthio)ethyl ester 7694-58-8, Acetic acid, (3,5-di-tert-butyl-4-hydroxyphenyl)-, 2-(octadecylthio)ethyl ester 15188-12-2, Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-, octadecyl ester 15229-59-1, Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-, hexyl ester **35455-13-1**, 1,2-Propanediol, bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate) **35455-13-1**, Hydrocinnamic acid, 3,5-di-tert-butyl-4-hydroxy-, propylene ester **38879-22-0**, Diethylene glycol, 3,5-di-tert-butyl-4-hydroxyhydrocinnamate **38879-22-0**, Hydrocinnamic acid, 3,5-di-tert-butyl-4-hydroxy-, diester with diethylene glycol 57006-81-2, Acetic acid, (3,5-di-tert-butyl-4-hydroxyphenyl)-, diester with 2,2'-thiodiethanol 94441-59-5, Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-, 2-[(2-hydroxyethyl)thio]ethyl ester

95869-37-7, Benzoic acid, 3,5-di-tert-butyl-4-hydroxy-, 2-(octylthio)ethyl ester 96808-83-2, Acetic acid, (3,5-di-tert-butyl-4-hydroxyphenyl)-, 2-(octylthio)ethyl ester
(preparation of)

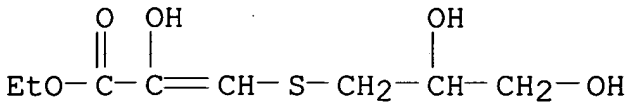
=> d l49 1-14 cbib abs hitstr hitind

L49 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2003:43045 Document No. 138:89499 Preparation of pyruvate derivatives for treating conditions characterized by oxidative stress. Wang, Bing; Miller, Guy; Zhang, Wei; Janagani, Satyanarayana; Song, Jiangao (USA). U.S. Pat. Appl. Publ. US 2003013847 A1 20030116, 54 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-138937 20020503. PRIORITY: US 2001-PV288649 20010503; US 2001-PV295314 20010601; US 2002-PV368456 20020323.

AB Pyruvate derivs. A-X-CH2COCO-Z and A-X-CH:C(OH)CO-Z [A = substituted alkyl or heteroaryl, heterocyclyl, (un)substituted nucleoside, di-, tri- or tetrapeptide, CH2COCO2R', or CH:C(OH)CO2R', where R' = H, (un)substituted (cyclo)alkyl or aryl; X = NR', S, SO, SO2, S-Y-S [Y = (un)substituted aryl, heteroaryl, nucleoside, amino acid, di, tri- or tetrapeptide], or a covalent bond to the sulfur atom of Cys or to the nitrogen atom of optionally substituted heterocyclyl; Z = OR or SR, where R = H, (un)substituted (cyclo)alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, or heterocycloalkyl] or their pharmaceutically-acceptable salts were prepared for treating a number of conditions characterized by oxidative stress. Certain known and novel pyruvate derivs. are particularly active in restoring or preserving metabolic integrity in oxidatively competent cells that have been subjected to oxygen deprivation. Thus, S-[3-(pentyloxy)-2,3-dioxopropyl]glutathione was prepared by alkylation of glutathione. Compds. of the invention were evaluated as agents for protection against ischemic damage.

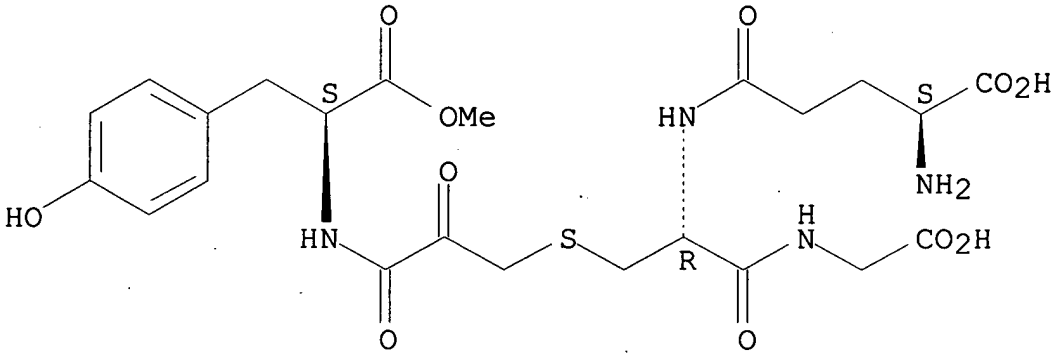
IT **475294-10-1P 475294-42-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

RN 475294-10-1 HCAPLUS
CN 2-Propenoic acid, 3-[(2,3-dihydroxypropyl)thio]-2-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



RN 475294-42-9 HCAPLUS
CN Glycine, L-γ-glutamyl-S-[3-[[(1S)-1-[(4-hydroxyphenyl)methyl]-2-methoxy-2-oxoethyl]amino]-2,3-dioxopropyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07K005-06
ICS C07C323-00; C07H019-16; C07H019-06; C07D293-10; C07D235-14
NCL 530330000; 530331000; 536027300; 536028400; 544162000; 544287000; 548121000; 548204000; 548304400; 548316400
CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 1, 34
IT 27784-53-8P 73472-98-7P 114669-82-8P 349444-96-8P
349445-15-4P 475293-79-9P 475293-80-2P 475293-81-3P
475293-82-4P 475293-83-5P 475293-84-6P 475293-85-7P
475293-86-8P 475293-87-9P 475293-88-0P 475293-89-1P
475293-90-4P 475293-91-5P 475293-92-6P 475293-93-7P
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475294-39-4P 475294-40-7P 475294-41-8P **475294-42-9P**
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475294-79-2P 475294-80-5P 475294-81-6P 475294-82-7P
475557-24-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

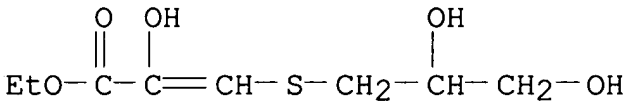
L49 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2003:43044 Document No. 138:89500 Preparation of pyruvate derivatives for treating conditions characterized by oxidative stress. Wang, Bing; Miller, Guy; Janagani, Satyanarayana; Zhang, Wei (USA). U.S. Pat. Appl. Publ. US 2003013846 A1 20030116, 55 pp., Cont.-in-part of U. S Provisional Ser. No. 368,456. (English). CODEN: USXXCO. APPLICATION: US 2002-138809 20020503. PRIORITY: US 2001-PV288649 20010503; US 2001-PV295314 20010601; US 2002-PV368456 20020323.

AB Pyruvate derivs. A-X-CH2C(:W)CONRbRc and A-X-CH:C(W)CONRbRc [A = (un)substituted (cyclo)alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, heterocycloalkyl, nucleoside, amino acid, di-, tri- or tetrapeptide, CH2COCO2R', or CH:C(OH)CO2R', where R' = H, (un)substituted (cyclo)alkyl or aryl; X = S, SO, SO2, S-Y-S [Y = (un)substituted aryl, heteroaryl, nucleoside, amino acid, di, tri- or tetrapeptide], or a covalent bond to the sulfur atom of Cys or to the nitrogen atom of optionally substituted heterocyclyl; W = :O, :NORa, or N(OH)Rd; Ra = H, (un)substituted alkyl, aryl, aralkyl, or alkenyl; Rb = H, (un)substituted (cyclo)alkyl, aryl, or aralkyl; Rc = H or (un)substituted alkyl; or RbRcN = 5- to 7-membered heterocyclyl; Rd = H, acyl, or (un)substituted alkyl] or their pharmaceutically-acceptable salts were prepared for treating a number of conditions characterized by oxidative stress. Certain known and novel pyruvate derivs. are particularly active in restoring or preserving metabolic integrity in oxidatively competent cells that have been subjected to oxygen deprivation. Thus, S-[3-(4-methylpiperidino)-2,3-dioxopropyl]glutathione was prepared via alkylation of glutathione. Compds. of the invention were evaluated as agents for protection against ischemic damage.

IT **475294-10-1P 475294-42-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP

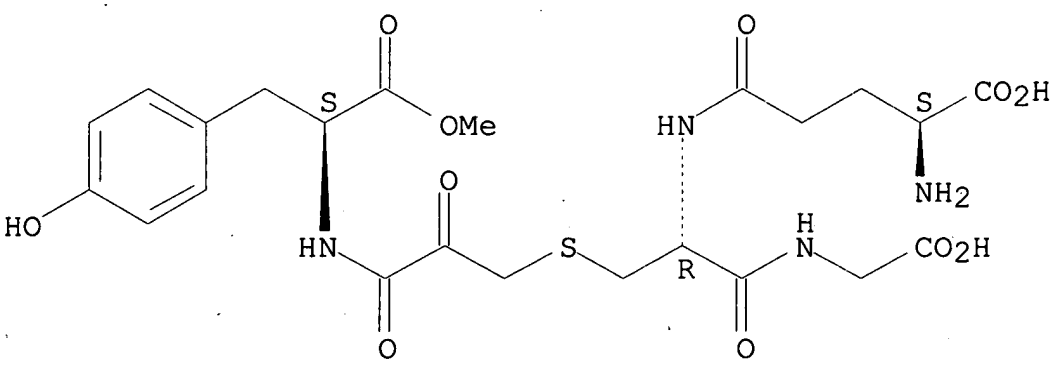
(Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

RN 475294-10-1 HCAPLUS
CN 2-Propenoic acid, 3-[(2,3-dihydroxypropyl)thio]-2-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



RN 475294-42-9 HCAPLUS
CN Glycine, L-γ-glutamyl-S-[3-[[(1S)-1-[(4-hydroxyphenyl)methyl]-2-methoxy-2-oxoethyl]amino]-2,3-dioxopropyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07K005-06
ICS C07H019-16; C07H019-048; C07D279-12; C07D277-60
NCL 530330000; 530331000; 536027230; 536028100; 540544000; 540575000; 540609000; 544059000; 544162000; 544402000
CC 23-18 (Aliphatic Compounds)
Section cross-reference(s): 1, 34
IT 27784-53-8P 73472-98-7P 114669-82-8P 349444-96-8P
349445-15-4P 475293-79-9P 475293-80-2P 475293-81-3P
475293-82-4P 475293-83-5P 475293-84-6P 475293-85-7P
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475294-02-1P 475294-03-2P 475294-04-3P 475294-05-4P
475294-06-5P 475294-07-6P 475294-08-7P 475294-09-8P

475294-10-1P 475294-11-2P 475294-12-3P 475294-14-5P
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475294-23-6P 475294-24-7P 475294-25-8P 475294-26-9P
475294-27-0P 475294-28-1P 475294-29-2P 475294-30-5P
475294-31-6P 475294-32-7P 475294-33-8P 475294-34-9P
475294-35-0P 475294-36-1P 475294-37-2P 475294-38-3P
475294-39-4P 475294-40-7P 475294-41-8P **475294-42-9P**
475294-43-0P 475294-44-1P 475294-45-2P 475294-46-3P
475294-47-4P 475294-48-5P 475294-49-6P 475294-60-1P
475294-63-4P 475294-64-5P 475294-65-6P 475294-66-7P
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475294-75-8P 475294-76-9P 475294-77-0P 475294-78-1P
475294-81-6P 475294-82-7P 475557-24-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

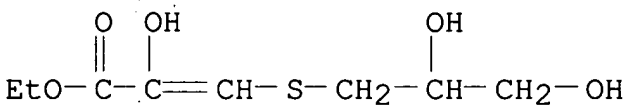
L49 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2003:43014 Document No. 138:73002 Preparation of pyruvate derivatives for treating conditions characterized by oxidative stress. Wang, Bing; Miller, Guy; Janagani, Satyanarayana (USA). U.S. Pat. Appl. Publ. US 2003013657 A1 20030116, 52 pp., Cont.-in-part of U. S. Provisional Ser. No. 368,456. (English). CODEN: USXXCO. APPLICATION: US 2002-138938 20020503. PRIORITY: US 2001-PV288649 20010503; US 2001-PV295314 20010601; US 2002-PV368456 20020323.

AB Pyruvate derivs. A-X-CH2C(:NORa)CO-Z [A = (un)substituted (cyclo)alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, heterocycloalkyl, nucleoside, amino acid, di-, tri- or tetrapeptide, CH2COCO2R', or CH:C(OH)CO2R', where R' = H, (un)substituted (cyclo)alkyl or aryl; X = S, SO, S-Y-S [Y = (un)substituted aryl, heteroaryl, nucleoside, amino acid, di-, tri- or tetrapeptide], or a covalent bond to the sulfur atom of Cys or to the nitrogen atom of optionally substituted heterocyclyl; Ra = H, (un)substituted alkyl , aryl, aralkyl, or alkenyl; Z = OR or SR, where R = (un)substituted (cyclo)alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, or heterocycloalkyl], including tautomers, stereoisomers, and mixts. of these, and their pharmaceutically-acceptable salts, were prepared for treating a number of conditions characterized by oxidative stress. Certain known and novel pyruvate derivs. are particularly active in restoring or preserving metabolic integrity in oxidatively competent cells that have been subjected to oxygen deprivation. Thus, S-[3-ethoxy-2-(hydroxyimino)-3-

oxopropyl]glutathione was prepared by alkylation of glutathione with 3-bromo-2-(hydroxyimino)propionic acid Et ester. Compds. of the invention were evaluated as agents for protection against ischemic damage.

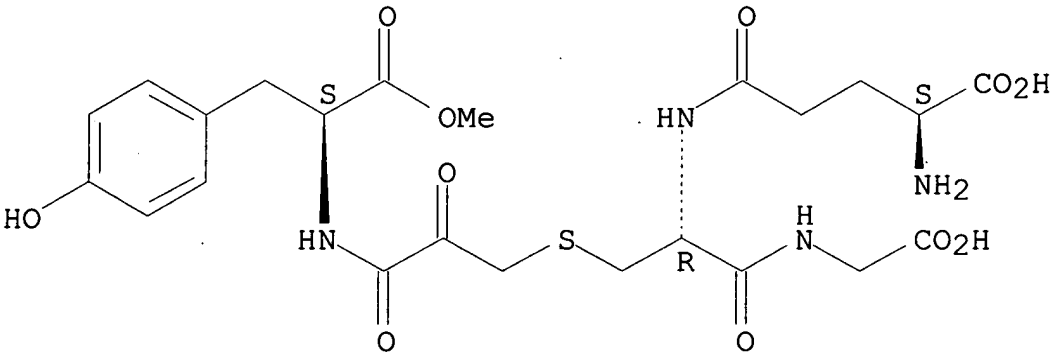
IT **475294-10-1P 475294-42-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

RN 475294-10-1 HCAPLUS
CN 2-Propenoic acid, 3-[(2,3-dihydroxypropyl)thio]-2-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



RN 475294-42-9 HCAPLUS
CN Glycine, L-γ-glutamyl-S-[3-[[(1S)-1-[(4-hydroxyphenyl)methyl]-2-methoxy-2-oxoethyl]amino]-2,3-dioxopropyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K038-08
ICS A61K038-06; A61K031-7076; A61K031-7072; A61K031-44; A61K031-401; A61K031-198
NCL 514017000; 514018000; 514019000; 514045000; 514049000; 514357000; 514408000; 514513000; 514551000; 514564000
CC 23-18 (Aliphatic Compounds)
Section cross-reference(s): 1, 34
IT 27784-53-8P 73472-98-7P 114669-82-8P 349444-96-8P

349445-15-4P 475293-79-9P 475293-80-2P 475293-81-3P
475293-82-4P 475293-83-5P 475293-84-6P 475293-85-7P
475293-86-8P 475293-87-9P 475293-88-0P 475293-89-1P
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475294-81-6P 475294-82-7P 475557-24-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

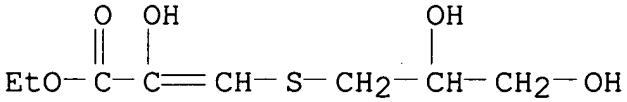
L49 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2003:43013 Document No. 138:73001 Preparation of pyruvate derivatives for treating conditions characterized by oxidative stress. Wang, Bing; Miller, Guy; Flaim, Stephen F.; Del Balzo, Ughetta; Zhang, Wei; Janagani, Satyanarayana; Song, Jiangao (USA). U.S. Pat. Appl. Publ. US 2003013656 A1 20030116, 56 pp. (English). CODEN: USXXCO. APPLICATION: US 2002-138726 20020503. PRIORITY: US 2001-PV288649 20010503; US 2001-PV295314 20010601; US 2002-PV368456 20020323.

AB Pyruvate derivs. A-X-CH2C(:W)CO-Z and A-X-CH:C(W)CO-Z [A = (un)substituted (cyclo)alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, heterocycloalkyl, nucleoside, amino acid, di-, tri- or tetrapeptide, CH2COCO2R', or CH:C(OH)CO2R', where R' = H, (un)substituted (cyclo)alkyl or aryl; X = NR', S, SO, SO2, S-Y-S [Y = (un)substituted aryl, heteroaryl, nucleoside, amino acid, di, tri- or tetrapeptide], or a covalent bond to the sulfur atom of Cys or to the nitrogen atom of optionally substituted heterocyclyl; W = :O, :NORa, :NNRbRc, or N(OH)Rd, where Ra = H, (un)substituted alkyl, aryl, aralkyl, or alkenyl; Rb

= H, (un)substituted (cyclo)alkyl, aryl, or aralkyl; Rc = H or (un)substituted alkyl; or RbRcN = 5- to 7-membered heterocyclyl; Rd = H, acyl, or (un)substituted alkyl; Z = OR, SR, or NRbRc, where R = (un)substituted (cyclo)alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, or heterocycloalkyl] or their pharmaceutically-acceptable salts were prepared for treating a number of conditions characterized by oxidative stress. Certain known and novel pyruvate derivs. are particularly active in restoring or preserving metabolic integrity in oxidatively competent cells that have been subjected to oxygen deprivation. Thus, 2-amino-4-[1-(carboxymethylcarbamoyl)-2-[2-oxo-2-(pentyloxycarbonyl)ethylsulfanyl]ethylcarbamoyl]butyric acid (claimed compound) was prepared from 3-bromopyruvic acid, pentanol, and glutathione.

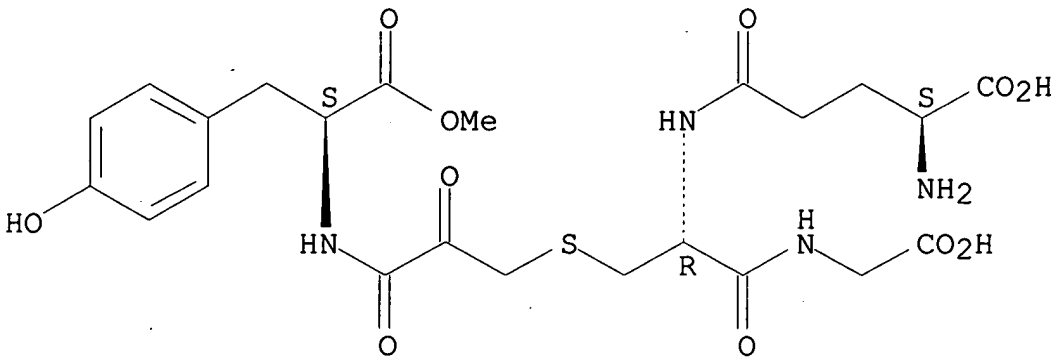
IT **475294-10-1P 475294-42-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

RN 475294-10-1 HCAPLUS
CN 2-Propenoic acid, 3-[(2,3-dihydroxypropyl)thio]-2-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



RN 475294-42-9 HCAPLUS
CN Glycine, L-γ-glutamyl-S-[3-[[(1S)-1-[(4-hydroxyphenyl)methyl]-2-methoxy-2-oxoethyl]amino]-2,3-dioxopropyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM A61K038-08
ICS A61K038-06; A61K031-7076; A61K031-7072; A61K031-198; A61K031-44; A61K031-40; A61K031-21
NCL 514017000; 514042000; 514045000; 514049000; 514357000; 514423000; 514513000; 514564000; 514626000
CC 23-18 (Aliphatic Compounds)
Section cross-reference(s): 1, 34
IT 27784-53-8P 73472-98-7P 114669-82-8P 349444-96-8P
349445-15-4P 475293-79-9P 475293-80-2P 475293-81-3P
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475294-81-6P 475294-82-7P 475557-24-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

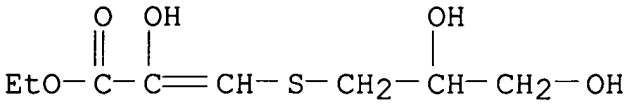
L49 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:868895 Document No. 137:369738 Preparation of pyruvate derivatives for treating conditions characterized by oxidative stress. Wang, Bing; Miller, Guy; Flaim, Stephen F.; Del Balzo, Ughetta; Zhang, Wei; Janagani, Satyanarayana; Song, Jingao (Galileo Laboratories, Inc., USA). PCT Int. Appl. WO 2002090314 A1 20021114, 143 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-US14057 20020503. PRIORITY: US 2001-PV288649 20010503; US 2001-PV295314 20010601; US 2002-PV368456 20020323.

AB Pyruvate derivs. A-X-CH2C(:W)CO-Z and A-X-CH:C(W)CO-Z [A = (un)substituted (cyclo)alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, heterocycloalkyl, nucleoside, amino acid, di-, tri- or tetrapeptide, CH2COCO2R', or CH:C(OH)CO2R', where R' = H, (un)substituted (cyclo)alkyl or aryl; X = NR', S, SO, SO2, S-Y-S [Y = (un)substituted aryl, heteroaryl, nucleoside, amino acid, di, tri- or tetrapeptide], or a covalent bond to the sulfur atom of Cys or to the nitrogen atom of optionally substituted heterocyclyl; W = :O, :NORa, :NNRbRc, or N(OH)Rd, where Ra = H, (un)substituted alkyl, aryl, aralkyl, or alkenyl; Rb = H, (un)substituted (cyclo)alkyl, aryl, or aralkyl; Rc = H or (un)substituted alkyl; or RbRcN = 5- to 7-membered heterocyclyl; Rd = H, acyl, or (un)substituted alkyl; Z = OR, SR, or NRbRc, where R = (un)substituted (cyclo)alkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, or heterocycloalkyl] or their pharmaceutically-acceptable salts were prepared for treating a number of conditions characterized by oxidative stress. Certain known and novel pyruvate derivs. are particularly active in restoring or preserving metabolic integrity in oxidatively competent cells that have been subjected to oxygen deprivation. Thus, 2-amino-4-[1-(carboxymethylcarbamoyl)-2-[2-oxo-2-(pentyloxycarbonyl)ethylsulfanyl]ethylcarbamoyl]butyric acid (claimed compound) was prepared from 3-bromopyruvic acid, pentanol, and glutathione.

IT **475294-10-1P 475294-42-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP

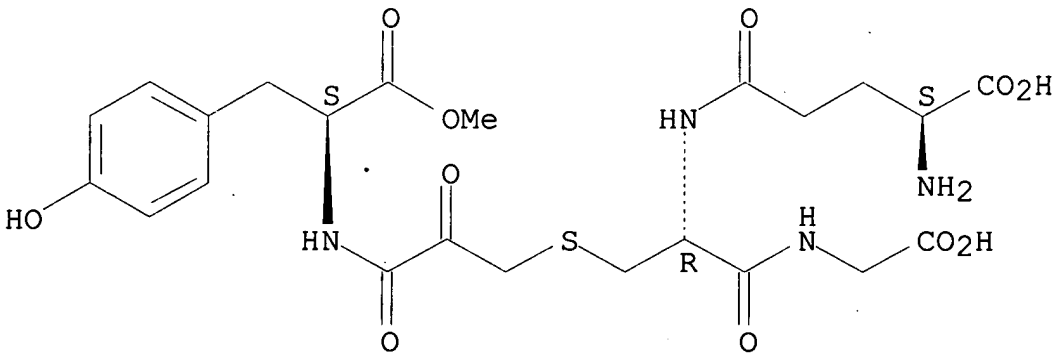
(Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

RN 475294-10-1 HCAPLUS
CN 2-Propenoic acid, 3-[(2,3-dihydroxypropyl)thio]-2-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



RN 475294-42-9 HCAPLUS
CN Glycine, L-γ-glutamyl-S-[3-[[(1S)-1-[(4-hydroxyphenyl)methyl]-2-methoxy-2-oxoethyl]amino]-2,3-dioxopropyl]-L-cysteinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IC ICM C07C069-66
ICS C07C323-60; C07D295-00; A61K031-12; A61K031-16; A61K031-215; A61K031-223; A61P009-10

CC 23-18 (Aliphatic Compounds)
Section cross-reference(s): 1, 34

IT 27784-53-8P 73472-98-7P 114669-82-8P 349444-96-8P
349445-15-4P 475293-79-9P 475293-80-2P 475293-81-3P
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475557-24-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyruvate derivs., including peptide derivs., for treating conditions characterized by oxidative stress)

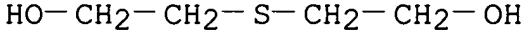
L49 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
2001:903775 Document No. 136:42534 Storage-stable compositions of glycerol monoalkyl ethers. Beilfuss, Wolfgang; Gradtke, Ralf (Air Liquide Sante (International), Fr.; Schuelke & Mayr G.m.b.H.). PCT Int. Appl. WO 2001093825 A1 20011213, 32 pp. DESIGNATED STATES: W: BR, JP, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-IB865 20010517. PRIORITY: DE 2000-10028638 20000609.

AB The present invention relates to compns. which comprise a combination (a) of 1 or more glycerol monoalkyl ethers, ROCH2CHOHCH2OH (where R= a branched or unbranched C3-18 alkyl, in which the alkyl group can be substituted by 1 or more hydroxyl and/or C1-4 alkoxy and/or the alkyl chain can be interrupted by up to 4 oxygen atoms), and (b) an antioxidant or 2 or more antioxidants as stabilizers, the simultaneous presence of phosphocholines and phosphocholine derivs. being excluded. 3-[(2-Ethylhexyl)oxy]-1,2-propanediol (Sensiva SC50) was mixed with a variety of substances, and the stability of the compns. during storage at room temperature in blue polyethylene bottles was tested. Following preparation of the samples, the value for ppm of H2O2 and the pH were determined at regular intervals. BHT, BHA, vitamin E and dexpanthenol stabilize the glycerol monoalkyl ethers over a long period, and in particular the appearance of peroxides, determined by the Merckoquant peroxide test, is avoided and as a result the neck-in effect is no longer observed when the antioxidants are

used.

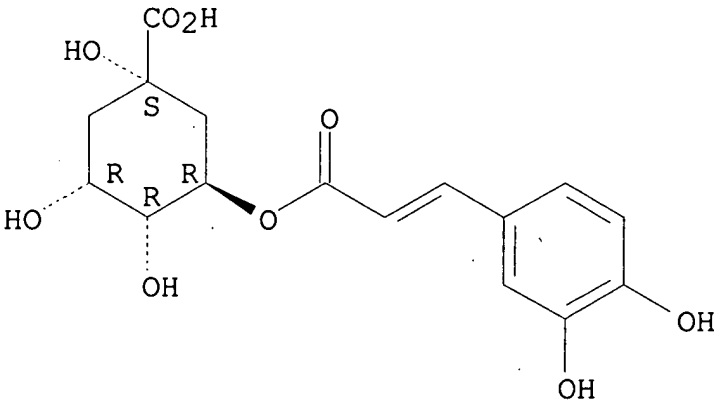
IT **111-48-8**, Thiodiglycol **327-97-9**, Chlorogenic acid **331-39-5**, Caffeic acid **1135-24-6**, Ferulic acid **4046-02-0**, Ethyl ferulate **20283-92-5**, Rosmarinic acid
RL: COS (Cosmetic use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(storage-stable compns. of glycerol monoalkyl ethers)

RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 327-97-9 HCAPLUS
CN Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, (1S,3R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



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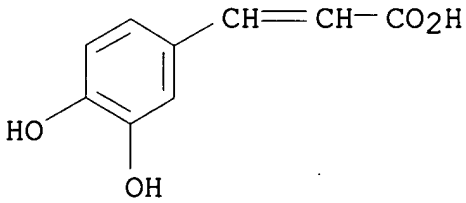
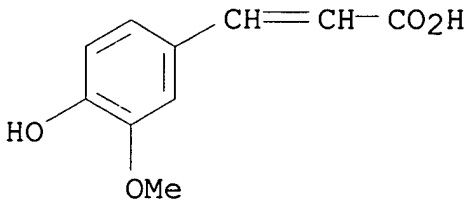
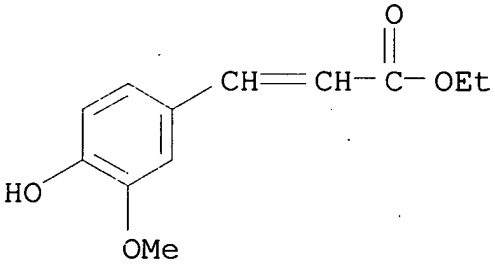


RN 1135-24-6 HCAPLUS
CN 2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)- (9CI) (CA INDEX NAME)

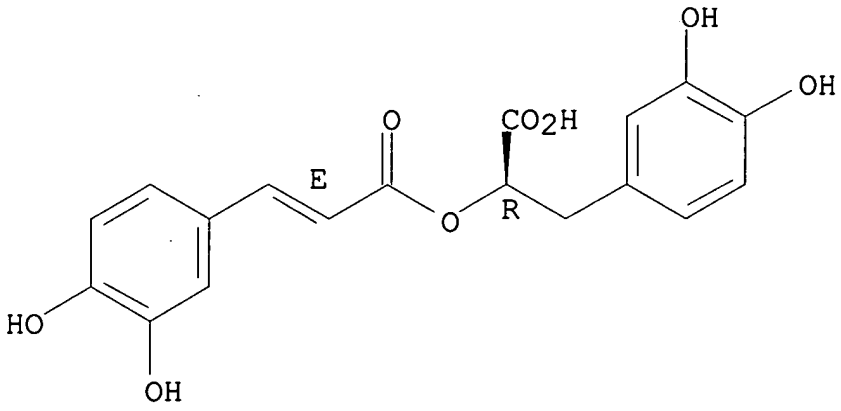


RN 4046-02-0 HCAPLUS
CN 2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 20283-92-5 HCAPLUS
CN Benzenepropanoic acid, α-[[(2E)-3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-3,4-dihydroxy-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IC ICM A61K007-48
ICS A61K007-40; A61K047-14; A61K047-18; A61K047-22; A61K047-10

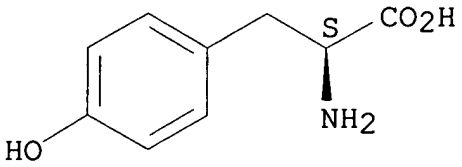
CC 62-4 (Essential Oils and Cosmetics)
Section cross-reference(s): 63

IT 50-21-5, Lactic acid, biological studies 52-89-1, Cysteine hydrochloride 52-90-4, Cysteine, biological studies 56-81-5D, Glycerol, monoalkyl ethers 58-95-7, Vitamin E acetate 68-11-1, Thioglycolic acid, biological studies 79-14-1, Glycolic acid, biological studies 79-42-5, Thiolactic acid 81-13-0, Dexpanthenol 89-65-6, Erythorbic acid 90-64-2, Mandelic acid 93-69-6, o-Tolylbiguanide 94-13-3, Propylparaben 94-26-8, Butylparaben 99-76-3, Methylparaben 99-96-7D, p-Hydroxybenzoic acid, esters 103-04-8, Phenylthioglycolic acid 108-73-6, Phloroglucinol **111-48-8**, Thiodiglycol 120-47-8, Ethylparaben 121-00-6, 3-tert-Butyl-4-hydroxyanisole 121-79-9, Propyl gallate 123-28-4, Dilauryl thiodipropionate 123-31-9, Hydroquinone, biological studies 123-93-3, Thiodiglycolic acid 128-37-0, 2,6-Di-tert-butyl-p-cresol, biological studies 150-76-5, p-Hydroxyanisole 153-18-4, Rutin **327-97-9**, Chlorogenic acid **331-39-5**, Caffeic acid 367-51-1, Sodium thioglycolate 499-44-5 500-38-9, Nordihydroguaiaretic acid 501-30-4, Kojic acid 616-91-1, Acetylcysteine 693-36-7, Distearyl thiodipropionate 1034-01-1, Octyl gallate **1135-24-6**, Ferulic acid 1166-52-5, Dodecyl gallate 1322-72-1, Di-tert-butylhydroquinone 1406-18-4, Vitamin E 1406-18-4D, Vitamin E, derivs. 1948-33-0, tert-Butylhydroquinone 3287-12-5, Dicetyl thiodipropionate **4046-02-0**, Ethyl ferulate 5470-11-1, Hydroxylamine hydrochloride 6381-77-7, Sodium erythorbate 6440-58-0 9002-96-4, Tocophersolan 10039-54-0, Hydroxylamine sulfate 10595-72-9 14246-53-8, Lipacide C8G 14618-65-6, Thiodiglycolamide 16545-54-3, Dimyristyl thiodipropionate 17048-39-4, Digalloyl trioleate **20283-92-5**, Rosmarinic acid 25103-09-7, Isooctyl

thioglycolate 26523-78-4, Tris(nonylphenyl)phosphite 34540-22-2 36148-84-2, Vitamin E linoleate 37311-39-0, Vitamin E succinate 43119-47-7, Vitamin E nicotinate 63947-37-5 70445-33-9, Sensiva SC50 74707-11-2 97692-61-0, Diamylhydroquinone 380151-83-7 380221-53-4
RL: COS (Cosmetic use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(storage-stable compns. of glycerol monoalkyl ethers)

L49 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1991:554155 Document No. 115:154155 A universal eluent system for free amino acid analysis in biological fluids. Pospisil, R.; Valik, D. (Dep. Biochem., Univ. Child. Hosp. J. G. Mendel, Brno, Czech.). Clinica Chimica Acta, 200(1), 49-51 (English) 1991. CODEN: CCATAR. ISSN: 0009-8981.
AB A universal eluent system is described for the anal. of free amino acids in biol. fluids, the basis of which is a single stock solution Analyses were performed using a Biotronik LC 7000 amino acid analyzer. The advantages of the eluent system involve namely efficient separation of free amino acids, cost effectiveness, reduced work load and good anal. precision.
IT **60-18-4**, Tyrosine, analysis
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in body fluids by cation-exchange liquid chromatog.
with universal eluent system)
RN 60-18-4 HCAPLUS
CN L-Tyrosine (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **111-48-8**, Thiodiglycol
RL: ANST (Analytical study)
(in amino acids determination in body fluids by cation-exchange liquid chromatog.)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

HO—CH_2—CH_2—S—CH_2—CH_2—OH

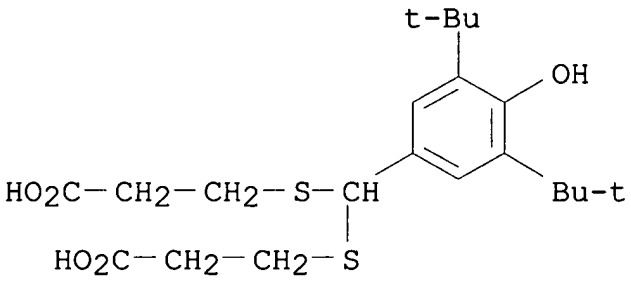
CC 9-3 (Biochemical Methods)
IT 56-12-2, 4-Aminobutyric acid, analysis 56-40-6, Glycine, analysis 56-41-7, Alanine, analysis 56-45-1, Serine, analysis 56-84-8, Aspartic acid, analysis 56-85-9, Glutamine, analysis 56-86-0, Glutamic acid, analysis 56-87-1, Lysine, analysis 56-88-2, Cystathionine 56-89-3, Cystine, analysis 57-13-6, Urea, analysis **60-18-4**, Tyrosine, analysis 61-90-5, Leucine, analysis 62-57-7, 2-Aminoisobutyric acid 63-68-3, Methionine, analysis 63-91-2, Phenylalanine, analysis 70-26-8, Ornithine 70-47-3, Asparagine, analysis 71-00-1, Histidine, analysis 72-18-4, Valine, analysis 72-19-5, Threonine, analysis 73-22-3, Tryptophan, analysis 73-32-5, Isoleucine, analysis 74-79-3, Arginine, analysis 107-35-7, Taurine 107-95-9, β-Alanine 141-43-5, Ethanolamine, analysis 147-85-3, Proline, analysis 332-80-9, 1-Methylhistidine 372-75-8, Citrulline 462-10-2 542-32-5, 2-Amino-adipic acid 1071-23-4, Phosphoethanolamine 2835-81-6, 2-Amino-butyric acid 7664-41-7, Ammonia, analysis 13100-82-8, Cysteic acid
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in body fluids by cation-exchange liquid chromatog.
with universal eluent system)
IT 109-86-4, Methylcellosolve **111-48-8**, Thiodiglycol 124-07-2, Caprylic acid, uses and miscellaneous 9002-92-0, Brij 35 7447-41-8, Lithium chloride (LiCl), uses and miscellaneous
RL: ANST (Analytical study)
(in amino acids determination in body fluids by cation-exchange liquid
chromatog.)

L49 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1990:180651 Document No. 112:180651 Stabilization of chlorine-containing resins against heat. Motohashi, Akira; Kogo, Yoshiyuki; Kizaki, Yoshio; Akitsu, Masaharu (Sankyo Organic Chemicals Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 01236252 A2 19890921 Heisei, 19 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1988-62704 19880316.
AB Adding organotin compds., thio ethers, and perchloric acid (I) or a salt to Cl-containing resins improves the resistance to heat. Roll kneading PVC 100, dibutyltin maleate 2.0, PhCH(SC2H4CO2H)2 0.05, and I 0.001 part gave 0.5-mm sheets with heat stability (195°) 75 min and good discoloration resistance during pressing of 8 sheets at 200° and 100 kg/cm2, vs. 50 and poor, resp., without I.

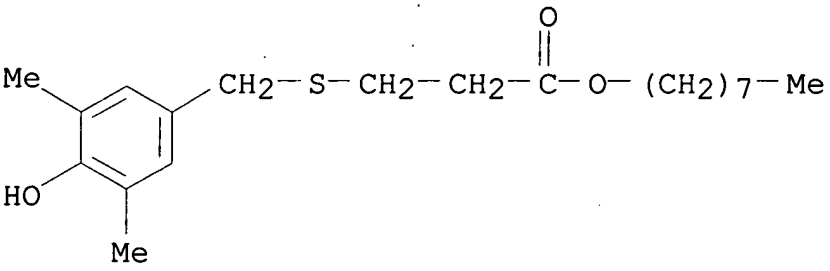
IT **111-48-8 88855-62-3 125703-55-1**
125703-57-3
RL: MOA (Modifier or additive use); USES (Uses)
(heat stabilizers, for chlorine-containing resins)

RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

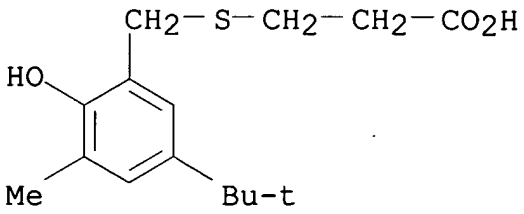
RN 88855-62-3 HCAPLUS
CN Propanoic acid, 3,3'-[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methylene]bis(thio)]bis- (9CI) (CA INDEX NAME)



RN 125703-55-1 HCAPLUS
CN Propanoic acid, 3-[[(4-hydroxy-3,5-dimethylphenyl)methyl]thio]-, octyl ester (9CI) (CA INDEX NAME)



RN 125703-57-3 HCAPLUS
CN Propanoic acid, 3-[[[5-(1,1-dimethylethyl)-2-hydroxy-3-methylphenyl]methyl]thio]- (9CI) (CA INDEX NAME)



IC ICM C08L027-04
ICS C08K005-57
CC 37-6 (Plastics Manufacture and Processing)
IT 77-58-7, Dibutyltin dilaurate 78-04-6, Dibutyltin maleate 78-06-8 78-20-6, Dibutyltin mercaptoacetate 111-17-1 **111-48-8** 123-28-4 1030-02-0 1185-81-5 1344-28-1D, Alumina, reaction products with perchloric acid 1344-95-2D, Calcium silicate, reaction products with perchloric acid 1462-52-8 4253-22-9 4265-55-8 4917-76-4 5587-52-0, Dibutyltin bis(cyclohexylmaleate) 6188-78-9 7324-74-5, Dibutyltin bis(benzylmaleate) 7429-90-5D, Aluminum, complexes with carboxyethyl thioethers 7601-89-0, Sodium perchlorate 7601-90-3, Perchloric acid, uses and miscellaneous 7631-86-9D, Silica, reaction products with perchloric acid 7695-69-4 7778-74-7, Potassium perchlorate 7790-98-9, Ammonium perchlorate 7791-03-9, Lithium perchlorate 10034-81-8, Magnesium perchlorate 10039-33-5, Dioctyltin bis(2-ethylhexylmaleate) 11097-59-9D, Isocalcite, reaction products with perchloric acid 13450-97-0, Strontium perchlorate 13465-95-7, Barium perchlorate 13477-36-6, Calcium perchlorate 13637-61-1, Zinc perchlorate 15546-12-0, Dibutyltin bis(2-ethylhexylmaleate) 15546-16-4, Dibutyltin bis(butylmaleate) 21645-51-2D, Aluminum hydroxide, reaction products with perchloric acid 25168-24-5, Dibutyltin bis(isooctylmercaptoacetate) 25253-54-7, Tin perchlorate 25852-70-4, Monobutyltin tris(isooctylmercaptoacetate) 26401-97-8, Dioctyltin bis(isooctylmercaptoacetate) 26636-01-1, Dimethyltin bis(isooctylmercaptoacetate) 26761-46-6, Dibutyltin bis(isooctyl-3-mercaptopropionate) 29881-72-9, Dibutyltin bis(oleyl maleate) 30232-12-3 37449-09-5 55348-64-6 57646-39-6 63397-60-4 68586-23-2 68687-20-7 69537-32-2 70518-72-8 71849-93-9 84030-61-5 85927-34-0 87441-93-8 **88855-62-3** 96841-64-4 98830-77-4 101023-92-1, Bis(dibutyltin methylmaleate)maleate 106226-73-7 123523-46-6 125679-59-6 125679-60-9 125679-61-0 125679-62-1 125679-63-2 125679-64-3 125679-65-4 125703-37-9 125703-38-0 125703-39-1 125703-40-4 125703-41-5 125703-42-6 125703-43-7 125703-44-8 125703-45-9 125703-46-0 125703-47-1 125703-48-2 125703-49-3 125703-50-6 125703-51-7 125703-52-8 125703-53-9

125703-54-0 **125703-55-1** 125703-56-2
125703-57-3 125703-58-4 125703-59-5 125703-60-8
125703-61-9 125703-62-0 125703-63-1 125703-64-2
125703-65-3 125703-66-4 125703-67-5 125728-83-8
125728-84-9 125920-95-8 126463-29-4
RL: MOA (Modifier or additive use); USES (Uses)
(heat stabilizers, for chlorine-containing resins)

L49 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1989:477645 Document No. 111:77645 Preparation of (3-phenylpropylthio)alkanoates and analogs as leukotriene antagonists. Wess, Guenther; Bartmann, Wilhelm; Beck, Gerhard; Anagnostopoulos, Hiristo (Hoechst A.-G., Fed. Rep. Ger.). Ger. Offen. DE 3724669 A1 19890202, 21 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1987-3724669 19870725.

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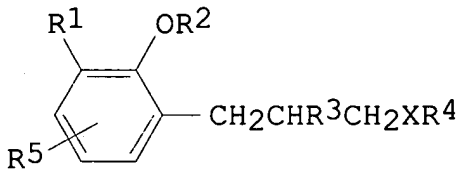
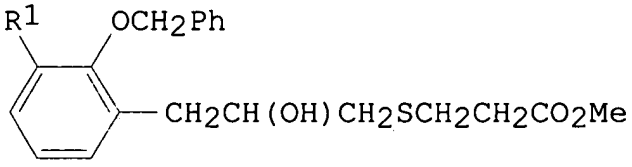


I



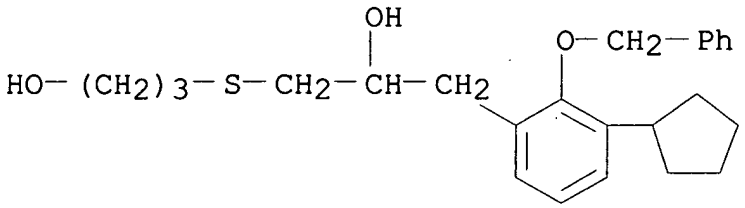
II

AB The title compds. [I; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, etc.; R2 = H, alkyl, pyridylmethyl, thienylmethyl, etc.; R3 = OH, OR6, OCOR7; R4 = alkyl, mono- or dihydroxyalkyl, alkoxyalkyl, etc.; R5 = H, halo, CF3, OH, alkyl, alkoxy; R6 = alkyl, allyl, PhCH2; R7 = alkyl, Ph; X = O, S, SO, SO2] were prepared 2-R1C6H4OCH2CH:CH2 (R1 = cyclopentyl) (preparation given) was heated at 220° for 4 h to give 3,2-R1(HO)C6H3CH2CH:CH2 which was refluxed 70 h with PhCH2Cl in Me2CO containing K2CO3 to give 3,2-R1(PhCH2O)C6H3CH2CH:CH2. The latter was stirred overnight with 3-ClC6H4CO2OH in CH2Cl2 to give (2-benzyloxy-3-cyclopentylbenzyl)oxirane which was stirred overnight with HSCH2CH2CO2Me to give title compound II (R1 = cyclopentyl). Similarly prepared II (R1 = H) had IC50 of 0.6-1.0, 0.6, and 0.6-1.0 μg/mL against LTC4, LTD4, and LTE4, resp., in vitro.

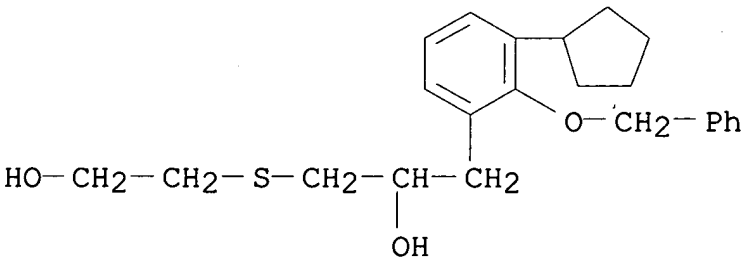
IT **119340-35-1P 122030-09-5P 122030-24-4P**

122030-36-8P 122030-38-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as leukotriene antagonist)

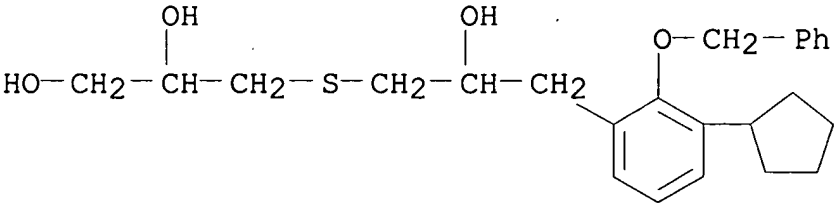
RN 119340-35-1 HCAPLUS
CN Benzeneethanol, 3-cyclopentyl-α-[[(3-hydroxypropyl)thio]methyl]-2-(phenylmethoxy)- (9CI) (CA INDEX NAME)



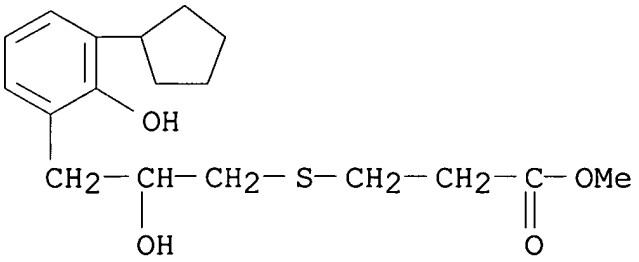
RN 122030-09-5 HCAPLUS
CN Benzeneethanol, 3-cyclopentyl-α-[[(2-hydroxyethyl)thio]methyl]-2-(phenylmethoxy)- (9CI) (CA INDEX NAME)



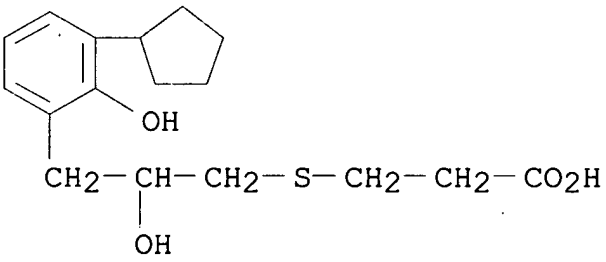
RN 122030-24-4 HCAPLUS
CN 1,2-Propanediol, 3-[[3-[3-cyclopentyl-2-(phenylmethoxy)phenyl]-2-hydroxypropyl]thio]- (9CI) (CA INDEX NAME)



RN 122030-36-8 HCAPLUS
CN Propanoic acid, 3-[[3-(3-cyclopentyl-2-hydroxyphenyl)-2-hydroxypropyl]thio]-, methyl ester (9CI) (CA INDEX NAME)



RN 122030-38-0 HCAPLUS
CN Propanoic acid, 3-[[3-(3-cyclopentyl-2-hydroxyphenyl)-2-hydroxypropyl]thio]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

IC ICM C07C149-273
ICS A61K031-215; A61K031-19; A61K031-44; A61K031-38; A61K031-41; C07C147-00; C07D317-36; C07D333-16; C07C043-00; C07D213-30; C07D295-18

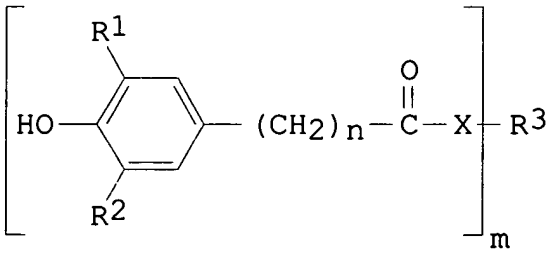
CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

IT 119340-32-8P 119340-34-0P **119340-35-1P** 119340-36-2P
119340-37-3P 119340-38-4P 119340-39-5P 119340-40-8P
119340-51-1P 119340-52-2P 122030-05-1P 122030-06-2P
122030-07-3P 122030-08-4P **122030-09-5P** 122030-23-3P
122030-24-4P 122030-25-5P 122030-26-6P 122030-27-7P
122030-28-8P 122030-29-9P 122030-30-2P 122030-31-3P

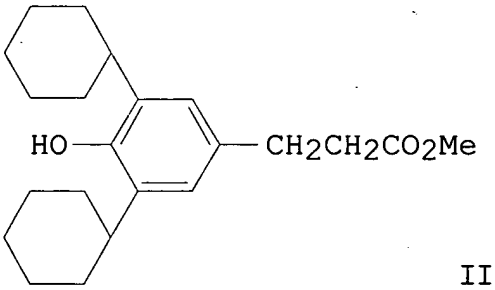
122030-32-4P 122030-33-5P 122030-34-6P 122030-35-7P
122030-36-8P 122030-38-0P 122030-39-1P
122030-40-4P 122030-41-5P 122030-42-6P 122030-43-7P
122030-44-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as leukotriene antagonist)

L49 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1987:458644 Document No. 107:58644 Substituted p-hydroxyphenyl compounds useful as antioxidants. Orban, Ivan; Meier, Hans Rudolf; Dubs, Paul; Evans, Samuel; Hofmann, Peter (Ciba-Geigy A.-G., Switz.). Eur. Pat. Appl. EP 219459 A2 19870422, 20 pp. DESIGNATED STATES: R: BE, DE, ES, FR, GB, IT, NL, SE. (German). CODEN: EPXXDW. APPLICATION: EP 1986-810441 19861006. PRIORITY: CH 1985-4399 19851011.

GI



I



II

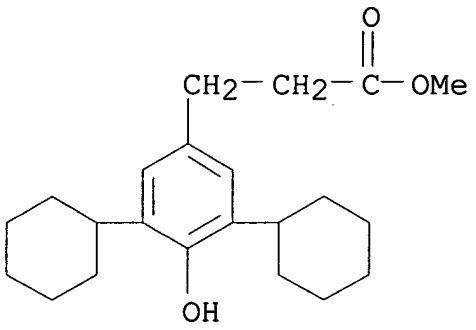
AB The title compds. [I; R1, R2 = (substituted) cycloalkyl or Ph, alkyl; X = O, NR4; n = 0-2; m = 1-4; R3 = alkyl, alkylene containing possible heteroatom interruption, etc.; R4 = H, alkyl, Ph], useful as antioxidants, are prepared A PhMe solution of 110.2 g octadecanol and 137.6 g Me (dicyclohexylhydroxyphenyl)propionate II was heated near reflux with subsequent azeotropic removal of MeOH to give I (R1 = R2 = cyclohexyl, R3 = n-C18H37, X = O, n = 2, m = 1), which at 0.1 weight % in combination with 0.3 weight % distearyl 3,3'-thiodipropionate (III) proved nearly 5 times more effective as an antioxidant for polypropylene than III alone.

IT **109276-49-5P 109276-59-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and transesterifications of)

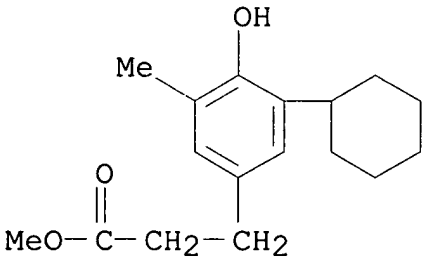
RN 109276-49-5 HCAPLUS

CN Benzenepropanoic acid, 3,5-dicyclohexyl-4-hydroxy-, methyl ester

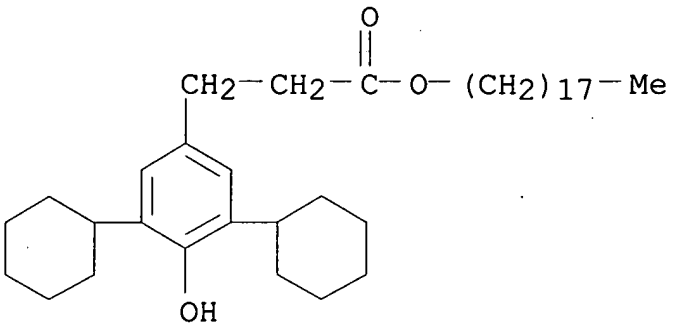
(9CI) (CA INDEX NAME)



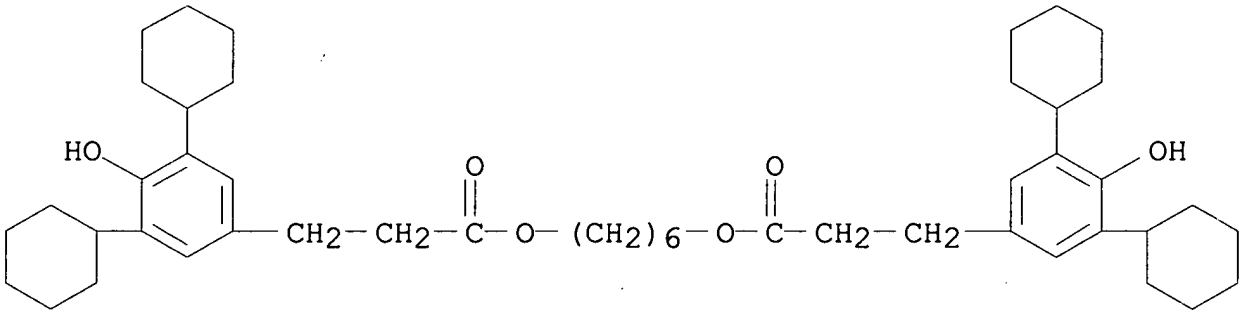
RN 109276-59-7 HCAPLUS
CN Benzenepropanoic acid, 3-cyclohexyl-4-hydroxy-5-methyl-, methyl ester (9CI) (CA INDEX NAME)



IT **109276-50-8P 109276-51-9P 109276-52-0P**
109276-54-2P 109276-55-3P 109276-56-4P
109276-57-5P 109276-58-6P 109333-58-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antioxidant)
RN 109276-50-8 HCAPLUS
CN Benzenepropanoic acid, 3,5-dicyclohexyl-4-hydroxy-, octadecyl ester (9CI) (CA INDEX NAME)

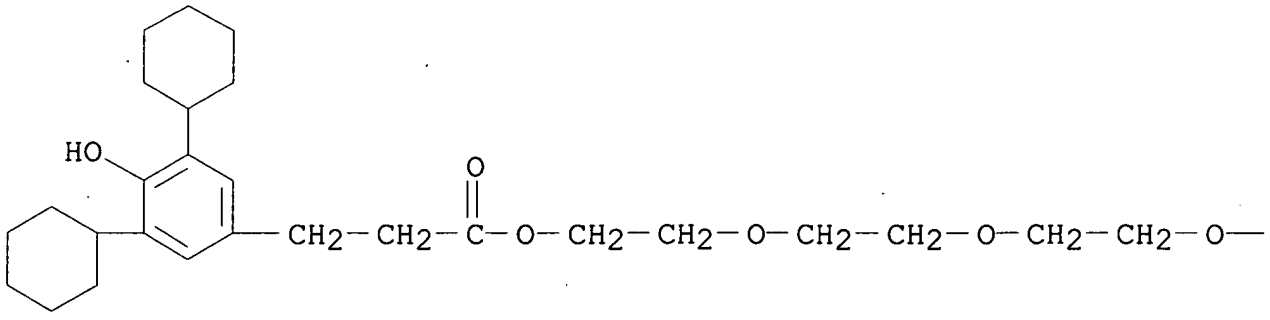


RN 109276-51-9 HCAPLUS
CN Benzenepropanoic acid, 3,5-dicyclohexyl-4-hydroxy-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)

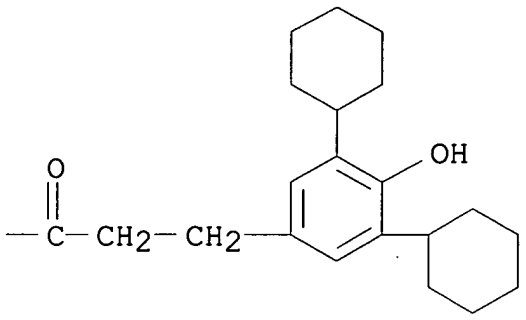


RN 109276-52-0 HCAPLUS
CN Benzenepropanoic acid, 3,5-dicyclohexyl-4-hydroxy-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester (9CI) (CA INDEX NAME)

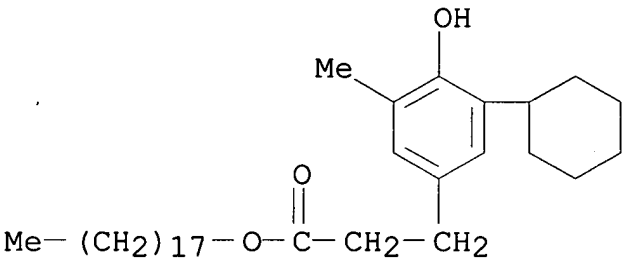
PAGE 1-A



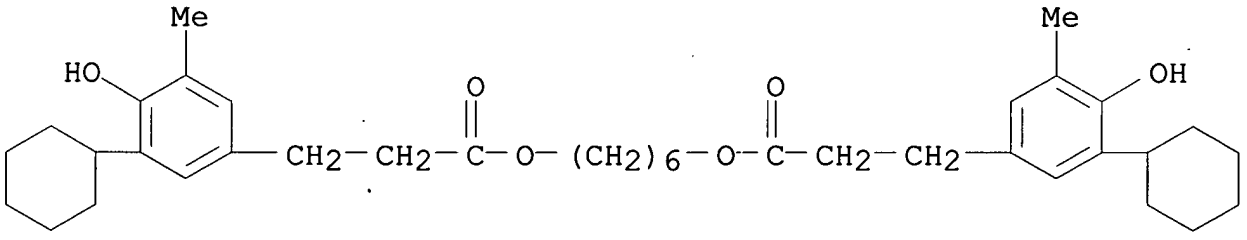
PAGE 1-B



RN 109276-54-2 HCAPLUS
CN Benzenepropanoic acid, 3-cyclohexyl-4-hydroxy-5-methyl-, octadecyl ester (9CI) (CA INDEX NAME)

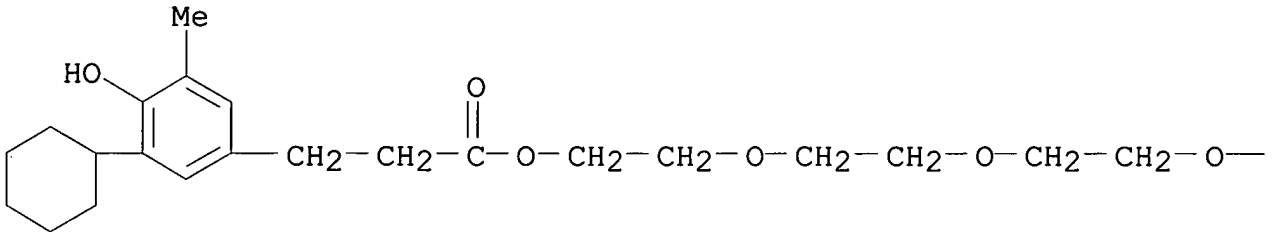


RN 109276-55-3 HCAPLUS
CN Benzenepropanoic acid, 3-cyclohexyl-4-hydroxy-5-methyl-, 1,6-hexanediyl ester (9CI) (CA INDEX NAME)

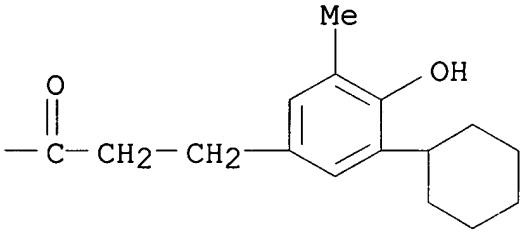


RN 109276-56-4 HCAPLUS
CN Benzenepropanoic acid, 3-cyclohexyl-4-hydroxy-5-methyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A

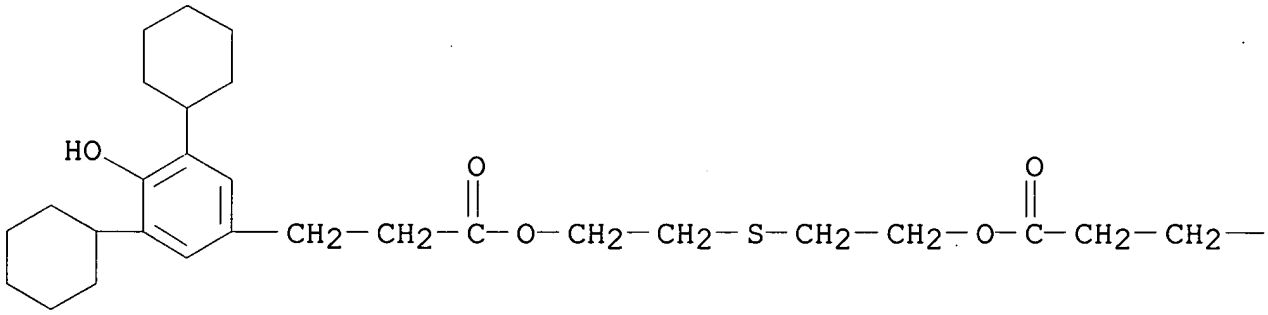


PAGE 1-B

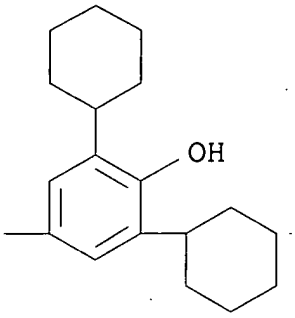


RN 109276-57-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-dicyclohexyl-4-hydroxy-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

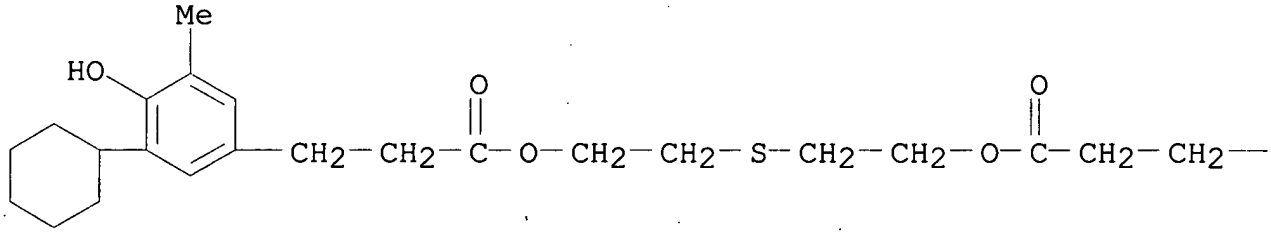


PAGE 1-B

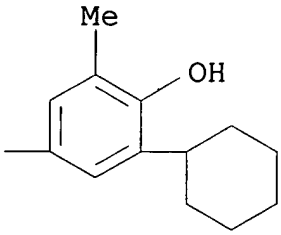


RN 109276-58-6 HCAPLUS
CN Benzenepropanoic acid, 3-cyclohexyl-4-hydroxy-5-methyl-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

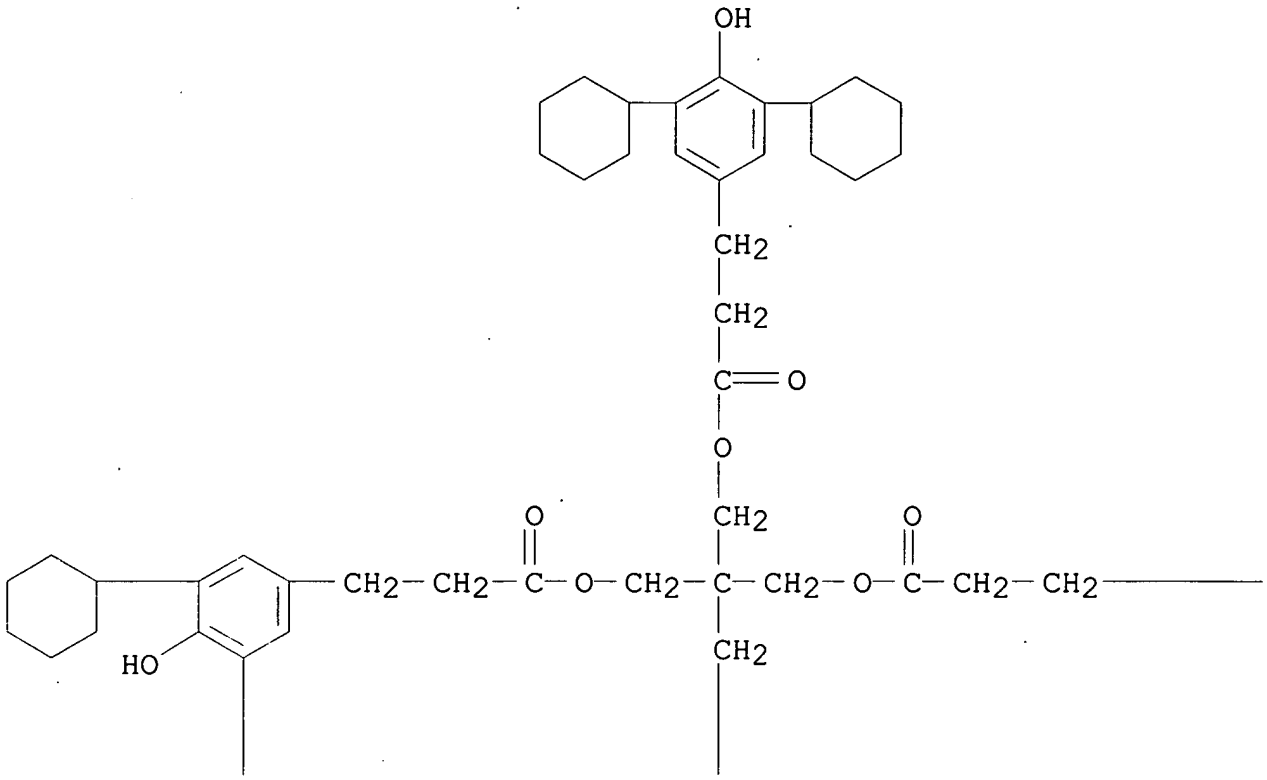


PAGE 1-B

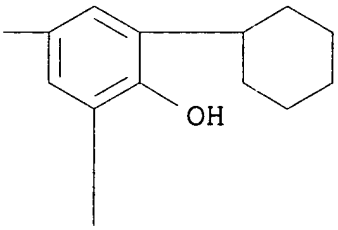


RN 109333-58-6 HCAPLUS
CN Benzenepropanoic acid, 3,5-dicyclohexyl-4-hydroxy-, 2,2-bis[[3-(3,5-dicyclohexyl-4-hydroxyphenyl)-1-oxopropoxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

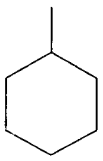
PAGE 1-A

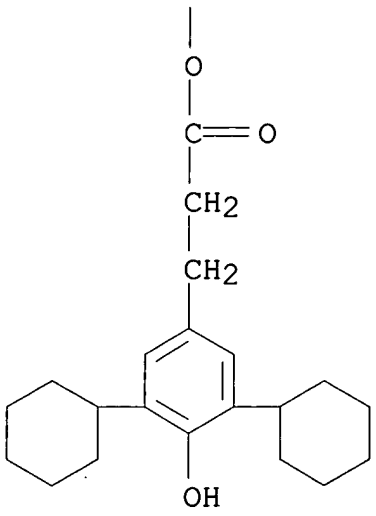


PAGE 1-B

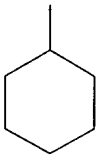


PAGE 2-A

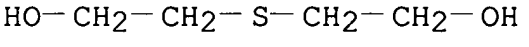




PAGE 2-B



IT **111-48-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(transesterification by, of Me hydroxyphenylpropionate derivative)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



IC ICM C07C069-732
ICS C07C103-76; C08K005-10; C07C149-20
CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 37
IT **109276-49-5P 109276-59-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and transesterifications of)
IT **109276-50-8P 109276-51-9P 109276-52-0P**
109276-53-1P **109276-54-2P 109276-55-3P**
109276-56-4P 109276-57-5P 109276-58-6P
109333-58-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antioxidant)
IT **111-48-8** 112-27-6, Triethyleneglycol 112-92-5
115-77-5, Pentaerythritol, reactions 629-11-8, 1,6-Hexanediol
RL: RCT (Reactant); RACT (Reactant or reagent)
(transesterification by, of Me hydroxyphenylpropionate derivative)

L49 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1985:488577 Document No. 103:88577 Analysis of technological mixtures of phenol antioxidants using reversed-phase liquid chromatography. Rubtsova, T. A.; Mel'nikova, N. A.; Chereshneva, A. F.; Glushkova, L. V. (Sci.-Res. Inst. Chem. Polym. Mater., Tambov, USSR). Zhurnal Analiticheskoi Khimii, 40(4), 721-4 (Russian) 1985. CODEN: ZAKHA8. ISSN: 0044-4502.
AB Transesterification products of Me β-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate (I) [**6386-38-5**] with pentaerythritol, diethylene glycol, or thiodiethylene glycol were

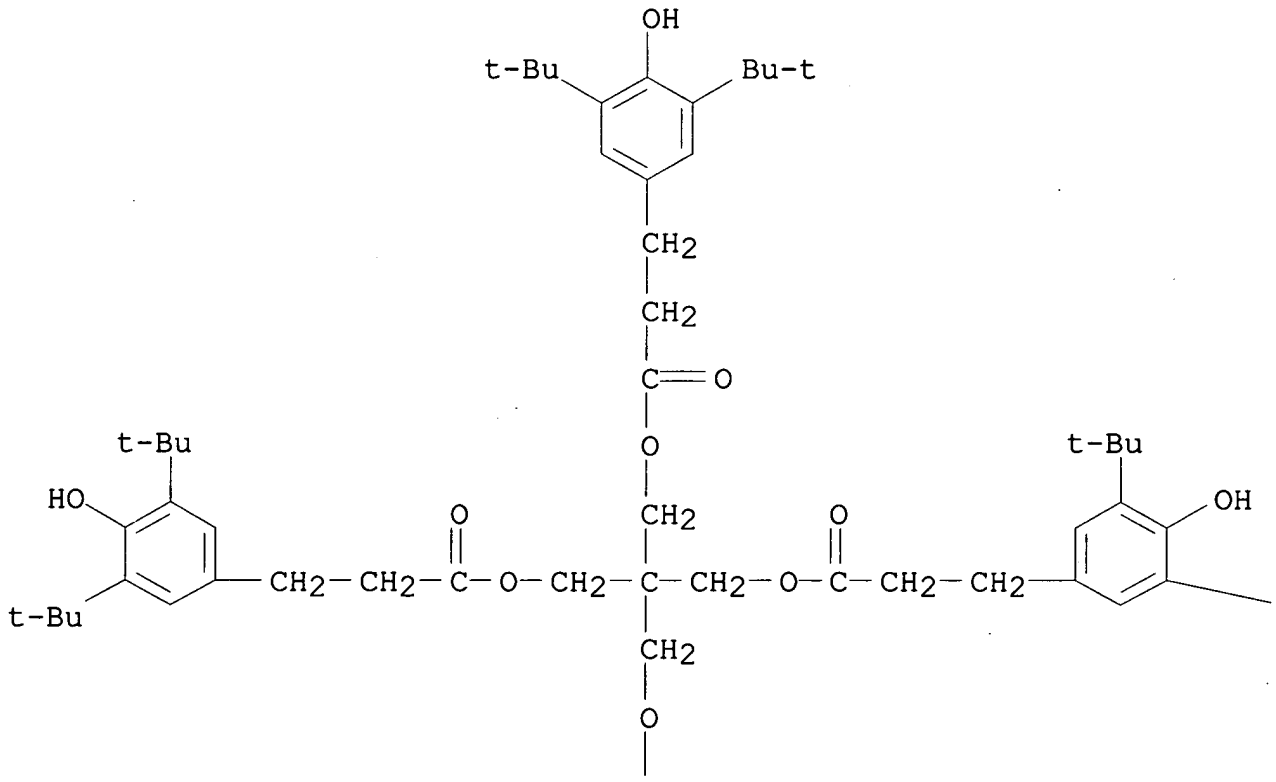
determined by reversed-phase, high-performance liquid chromatog. using octadecyl-functional column packing MSN-10 and H2O-dioxane eluents. The products contained com. antioxidants Fenozan 23 [**6683-19-8**], Fenozan 28 [**38879-22-0**], or Fenozan 30 [**41484-35-9**], comprising full esters, as well as lower esters, I, and unidentified compds.

IT **6683-19-8 38879-22-0 41484-35-9**
RL: USES (Uses)
(antioxidants, determination of, in transesterification products, by reversed-phase high-performance liquid chromatog.)

RN 6683-19-8 HCAPLUS

CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2,2-bis[[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy]methyl]-1,3-propanediyl ester (9CI) (CA INDEX NAME)

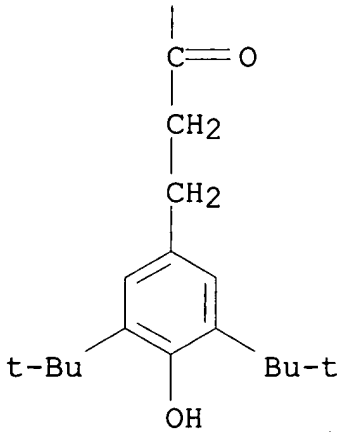
PAGE 1-A



PAGE 1-B

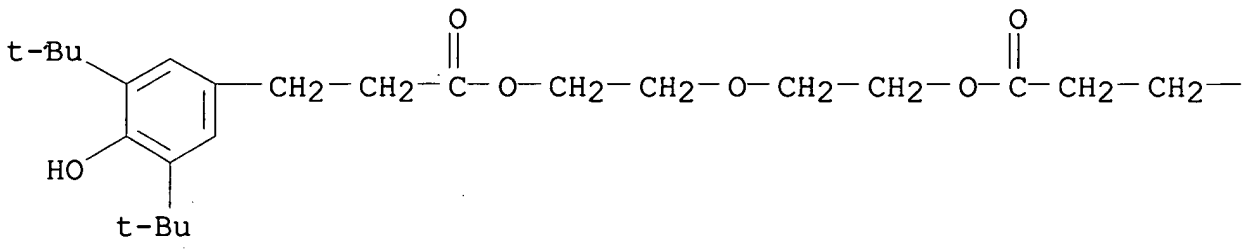
Bu-t

PAGE 2-A

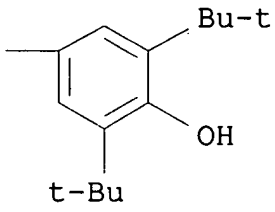


RN 38879-22-0 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, oxydi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

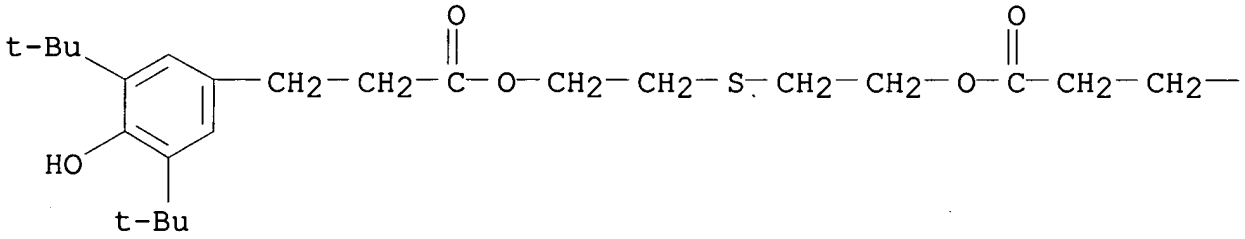


PAGE 1-B

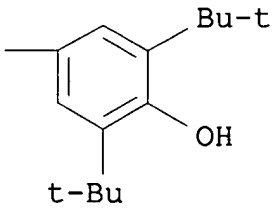


RN 41484-35-9 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, thiodi-2,1-ethanediyl ester (9CI) (CA INDEX NAME)

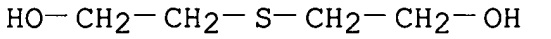
PAGE 1-A



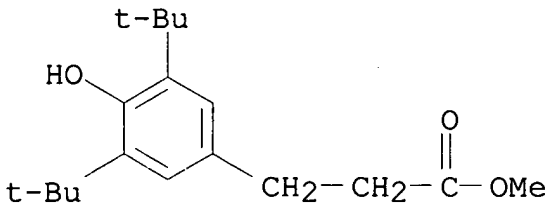
PAGE 1-B



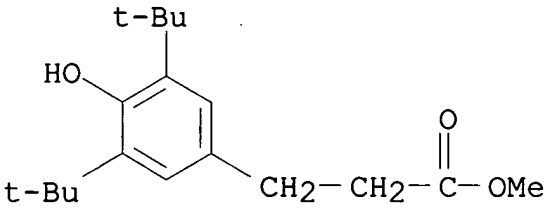
IT **111-48-8D**, reaction products with Me (dibutylhydroxyphenyl)propionate **6386-38-5D**, reaction products with polyols
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by reversed-phase high-performance liquid chromatog.)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)



RN 6386-38-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



IT **6386-38-5**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in transesterification products, by reversed-phase high-performance liquid chromatog.)
RN 6386-38-5 HCAPLUS
CN Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



CC 37-6 (Plastics Manufacture and Processing)
Section cross-reference(s): 80
IT **6683-19-8 38879-22-0 41484-35-9**
RL: USES (Uses)

(antioxidants, determination of, in transesterification products, by
reversed-phase high-performance liquid chromatog.)
IT 111-46-6D, reaction products with Me (dibutylhydroxyphenyl)propion ate **111-48-8D**, reaction products with Me (dibutylhydroxyphenyl)propionate 115-77-5D, reaction products with Me (dibutylhydroxyphenyl)propionate **6386-38-5D**, reaction products with polyols
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by reversed-phase high-performance liquid chromatog.)
IT **6386-38-5**
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in transesterification products, by reversed-phase
high-performance liquid chromatog.)

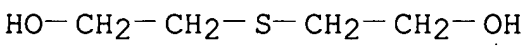
L49 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1985:20569 Document No. 102:20569 Triple-column ion-exchange physiological amino acid analysis with fluorescent detection: baseline characterization of human cerebrospinal fluid. Ferraro, Thomas N.; Hare, Theodore A. (Jefferson Med. Coll., Thomas Jefferson Univ., Philadelphia, PA, 19107, USA). Analytical Biochemistry, 143(1), 82-94 (English) 1984. CODEN: ANBCA2. ISSN: 0003-2697.
AB A highly resolving triple-column amino acid analyzer with fluorometric detection is described. The reliability of this technique was evaluated and it was used in a baseline investigation of amino acids and related compds. in human cerebrospinal fluid (CSF). The procedure employs 3 distinct ion-exchange columns to elute the acidic, neutral, and basic amino acids, resp. Each column is run isocratically with Li citrate buffers designed to provide overlapping elution profiles. Studies using CSF collected under strictly controlled conditions documented nanomolar concns. of aspartate, GABA, β-alanine, 1-methylhistidine, and 3-methylhistidine, as well as low levels of glutamate, methyllysine, and NH3. In addition, other common amino acids were also quantified. Chromatograms of CSF from all 3 systems (acidic, neutral, and basic) exhibited numerous uncharacterized compds. emphasizing the resolution and sensitivity of the anal. procedure. In vitro stability studies revealed that levels of aspartate, glutamate, GABA, homocarnosine, and NH3 are subject to significant change when CSF is maintained at room temperature
for various periods of time up to 24 h. Thus, the valid and accurate measurement of CSF amino compds., especially the neurotransmitter amino acids, requires a highly specific and sensitive assay procedure as well as strict control of CSF

manipulation in vitro.

IT **111-48-8**
RL: ANST (Analytical study)
(buffer containing, for amino acids determination in human cerebrospinal
fluid by ion-exchange HPLC with triple column and fluorometry)

RN 111-48-8 HCAPLUS

CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

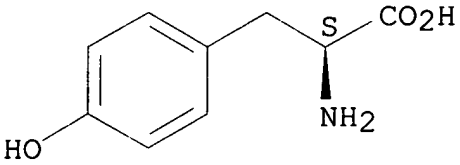


IT **60-18-4**, analysis
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in cerebrospinal fluid of humans by ion-exchange HPLC with triple column and fluorometry)

RN 60-18-4 HCAPLUS

CN L-Tyrosine (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CC 9-3 (Biochemical Methods)

IT **111-48-8** 124-07-2, uses and miscellaneous 77-92-9, uses and miscellaneous 7447-41-8, uses and miscellaneous
RL: ANST (Analytical study)
(buffer containing, for amino acids determination in human cerebrospinal
fluid by ion-exchange HPLC with triple column and fluorometry)

IT 56-12-2, analysis 56-40-6, analysis 56-41-7, analysis 56-45-1, analysis 56-84-8, analysis 56-85-9, analysis 56-86-0, analysis 56-87-1, analysis **60-18-4**, analysis 61-90-5, analysis 63-68-3, analysis 63-91-2, analysis 70-26-8 70-47-3, analysis 71-00-1, analysis 72-18-4, analysis 72-19-5, analysis 73-22-3, analysis 73-32-5, analysis 74-79-3, analysis 107-35-7 107-95-9 141-43-5, analysis 332-80-9 368-16-1 372-75-8 1071-23-4 1188-07-4 2835-81-6 3650-73-5 7664-41-7, analysis
RL: ANT (Analyte); ANST (Analytical study)
(determination of, in cerebrospinal fluid of humans by ion-exchange HPLC with triple column and fluorometry)

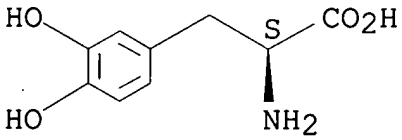
L49 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1983:466957 Document No. 99:66957 Fluorometric determination of secondary amines by high-performance liquid chromatography with post-column derivatization. Himuro, Akira; Nakamura, Hiroshi; Tamura, Zenzo (Fac. Pharm. Sci., Univ. Tokyo, Tokyo, 113, Japan). Journal of Chromatography, 264(3), 423-33 (English) 1983. CODEN: JOCRAM. ISSN: 0021-9673.

AB The title procedure was used for the simultaneous determination of primary and secondary amines. The postcolumn derivatization method is based on the manual procedure of A. Himuro et al. (1983) for secondary amines determination; secondary amines were converted to primary amines with NaOCl, and then primary amines were derivatized with o-phthalaldehyde-2-mercaptoethanol reagent with excess NaOCl suppressed by 2,2'-thiodiethanol. This conversion-derivatization-fluorometric detection method was studied for typical secondary amines and analogous primary amines by flow-injection anal. to find the optimum conditions. The conditions established for the postcolumn derivatization were applied to the determination of amino acids including L-proline and L-4-hydroxyproline as well as N-Me amino acids, catecholamines, and their 3-O-Me derivs.

IT **59-92-7**, analysis
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by high-performance liquid chromatog. with postcolumn derivatization and fluorometric detection)

RN 59-92-7 HCAPLUS
CN L-Tyrosine, 3-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **111-48-8**
RL: ANST (Analytical study)
(in secondary amines determination by liquid chromatog. and fluorometry)

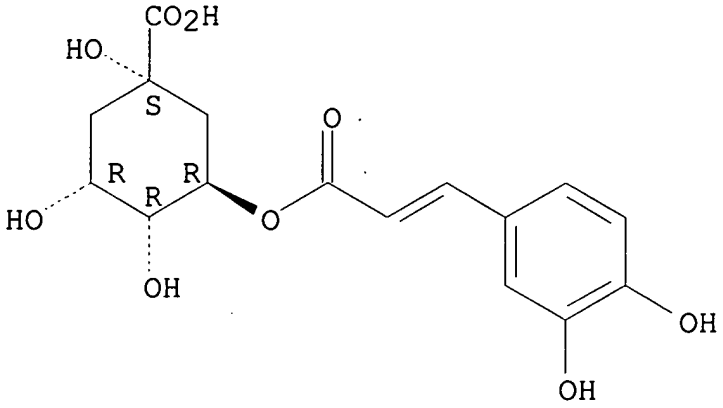
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

HO—CH_2—CH_2—S—CH_2—CH_2—OH

CC 9-3 (Biochemical Methods)
Section cross-reference(s): 2, 80
IT 51-35-4 51-41-2 51-43-4 51-61-6, analysis 56-12-2, analysis 56-41-7, analysis 56-84-8, analysis 56-87-1, analysis **59-92-7**, analysis 72-18-4, analysis 74-89-5, analysis 97-31-4 107-97-1 147-85-3, analysis 3060-46-6 5001-33-2
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by high-performance liquid chromatog. with postcolumn
derivatization and fluorometric detection)
IT **111-48-8** 7681-52-9
RL: ANST (Analytical study)
(in secondary amines determination by liquid chromatog. and fluorometry)

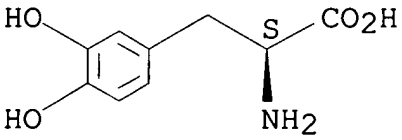
L49 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2005 ACS on STN
1977:454800 Document No. 87:54800 Enzymic color formation in beet and cane juices. Gross, D.; Coombs, J. (Group Res. Dev., Tate and Lyle Ltd., Reading/Berks., UK). C. R. Assem. Gen. Comm. Int. Tech. Sucr., 15th, 295-308. Comm. Int. Tech. Sucr.: Tienen, Belg. (English) 1975. CODEN: 35VOAL.
AB Polyphenoloxidase (I) [9002-10-2] with mol. wts. of 200,000 and 32,000-130,000, which catalyze the browning reactions during extraction
and refining of sugar, were isolated from sugar beet and cane juices, resp. and characterized for Michaelis constant and UV light maximum absorption for caffeic and chlorogenic acid (II), and 3,4-dihydroxyphenylalanine. The possible routes of color formation from II-mediated reactions involving the oxidation of a 2nd phenol or the reactions with amino acids or amino groups of proteins are given. Of the many chemical compds. tested, thioglycolate and β-mercaptoethanol [60-24-2] were the most effective compds. to inactivate the I.
IT **327-97-9**
RL: USES (Uses)
(colorant formation in presence of caffeic acid and, in sugar cane juices)
RN 327-97-9 HCAPLUS
CN Cyclohexanecarboxylic acid, 3-[[3-(3,4-dihydroxyphenyl)-1-oxo-2-propenyl]oxy]-1,4,5-trihydroxy-, (1S,3R,4R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

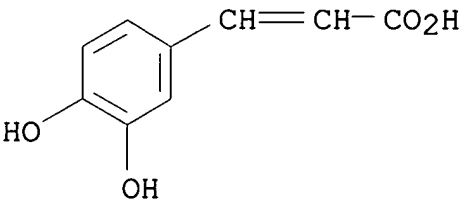


IT **59-92-7**, uses and miscellaneous **331-39-5**
RL: USES (Uses)
(colorant formation in presence of chlorogenic acid and, in sugar cane juices)
RN 59-92-7 HCAPLUS
CN L-Tyrosine, 3-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 331-39-5 HCAPLUS
CN 2-Propenoic acid, 3-(3,4-dihydroxyphenyl)- (9CI) (CA INDEX NAME)



IT **111-48-8**
RL: USES (Uses)
(inactivation by, of color forming polyphenoloxidase, in sugar beet and cane juices)
RN 111-48-8 HCAPLUS
CN Ethanol, 2,2'-thiobis- (9CI) (CA INDEX NAME)

HO—CH_2—CH_2—S—CH_2—CH_2—OH

CC 44-1 (Industrial Carbohydrates)
Section cross-reference(s): 16

IT **327-97-9**
RL: USES (Uses)
(colorant formation in presence of caffeic acid and, in sugar cane juices)

IT **59-92-7**, uses and miscellaneous 87-66-1 120-80-9, uses and miscellaneous **331-39-5** 569-77-7
RL: USES (Uses)
(colorant formation in presence of chlorogenic acid and, in sugar cane juices)

IT 50-81-7D, salt 52-90-4, uses and miscellaneous 60-00-4, uses and miscellaneous 60-24-2 68-11-1D, salt 70-18-8, uses and miscellaneous 70-49-5D, salt 96-27-5 **111-48-8** 140-89-6 147-84-2D, salt 2444-37-3D, salt 3483-12-3 6892-68-8 7681-57-4 9003-39-8 25322-68-3 30232-12-3D, salt
RL: USES (Uses)
(inactivation by, of color forming polyphenoloxidase, in sugar beet and cane juices)